

\mathcal{PT} -symmetry and Schrödinger operators. The double well case

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Abstract

We study a class of \mathcal{PT} -symmetric semiclassical Schrödinger operators, which are perturbations of a selfadjoint one. Here, we treat the case where the unperturbed operator has a double-well potential. In the simple well case, two of the authors have proved in [6] that, when the potential is analytic, the eigenvalues stay real for a perturbation of size $\mathcal{O}(1)$. We show here, in the double-well case, that the eigenvalues stay real only for exponentially small perturbations, then bifurcate into the complex domain when the perturbation increases and we get precise asymptotic expansions. The proof uses complex WKB-analysis, leading to a fairly explicit quantization condition.

Contents

1	Introduction and results	3
2	The complex WKB method	13
3	WKB analysis near a simple turning point	16
4	WKB solutions near the wells	20
5	WKB expansions of L^2 solutions outside the well	27
6	The quantization condition	33
7	The behaviour of the eigenvalues	40

1 Introduction and results

Operators that are \mathcal{PT} -symmetric have been proposed in quantum mechanics as an alternative to selfadjoint ones. From a physicist point of view, it is of course very important to verify that the spectrum of such operators is real and there has been a considerable activity in this area [1], [2], [3], [4], [7], [10], [9], [11], [15], [17], [18], [19], [20], [22], [21], [25]... There is in particular an issue [5] of the Journal of Physics A which is devoted to non-selfadjoint operators in quantum physics, where the \mathcal{PT} -symmetry property plays the main role. In a recent paper [8], E. Caliceti and S. Graffi study qualitatively if, in a perturbative setting, the phenomenon called \mathcal{PT} -symmetry phase transition occurs for \mathcal{PT} -symmetric polynomial potentials, that is if the eigenvalues bifurcate from real to complex values. The reader may also find interesting references in that paper.

It has been proved recently by two of the authors in [6] in the analytic category, that the \mathcal{PT} -symmetric perturbation of a semiclassical Schrödinger operator with a real-valued single well potential, have real spectrum even for perturbations of size $\mathcal{O}(1)$. Here we address the double-well case, where numerical results suggest that the situation is very different. For example, in Figure 1, we have plotted the eigenvalues of the Schrödinger operator $P_{\varepsilon,h} = h^2 D^2 + 0.05x^4 - .5x^2 + i\varepsilon x$ in a neighborhood of the barrier top, for $h = .01$ and $\varepsilon = k \cdot 10^{-m}$, $k = 1, 2, 3, 4$ and $m = 2, 3, 4, 5$. They have been computed by a simple finite difference scheme using the package `scipy` in python, and plotted using the package `matplotlib` [14]. It appears that the eigenvalues close to $E_0 > 0$ are real, giving a numerical illustration of the results in [6] since we are then in a simple well situation. In the double well case, that is for $E_0 < 0$, the eigenvalues close to E_0 seem to be non-real except for extremely small ε , and this is the phenomenon we consider in this paper.

We recall that an operator is said to be \mathcal{PT} -symmetric when it commutes with the operator \mathcal{PT} , where \mathcal{P} is the parity operator, and \mathcal{T} the time-reversal operator given by

$$(1.1) \quad \mathcal{P}u(x) = u(-x) \text{ and } \mathcal{T}u(x) = \overline{u(\bar{x})}.$$

Here, we study small perturbations $P_{h,\varepsilon} = P_\varepsilon(x, hD)$ of self-adjoint semi-

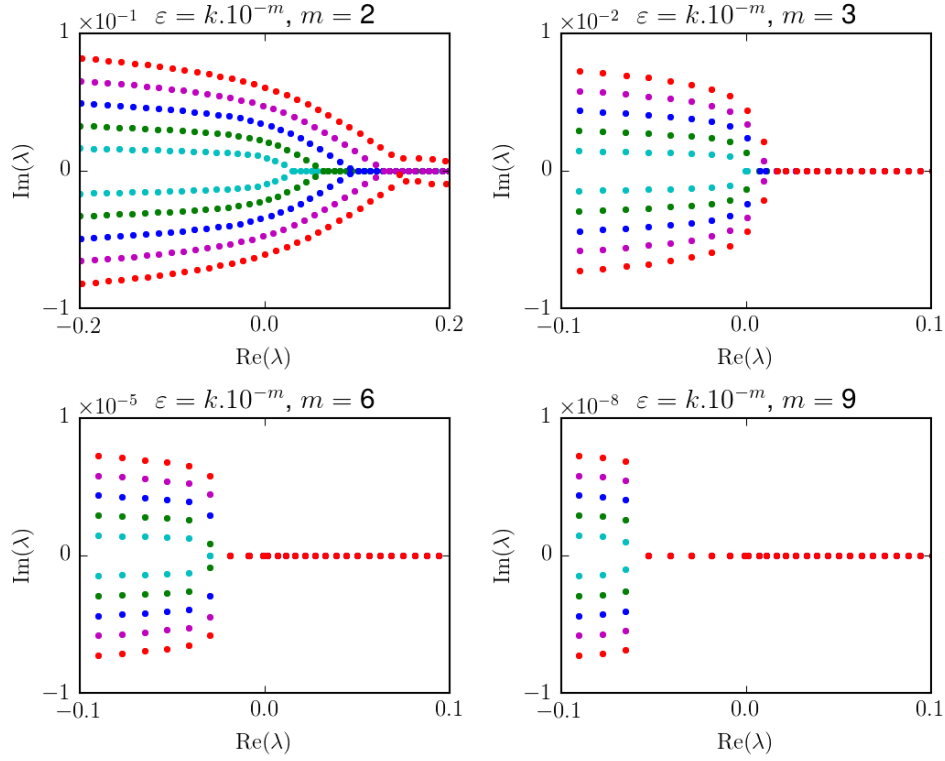


Figure 1: Eigenvalues of $P_{\epsilon,h} = h^2 D^2 + 0.05x^4 - .5x^2 + i\epsilon x$ near 0, with $h = 10^{-2}$ and $\epsilon = k \cdot 10^{-m}, k = 1, \dots, 5$.

classical Schrödinger operators of the form

$$(1.2) \quad P_\epsilon(x, hD) = -h^2 \frac{d^2}{dx^2} + V_\epsilon(x), \quad V_\epsilon(x) = V_0(x) + i\epsilon W(x),$$

where V_0 and W are smooth functions on \mathbb{R} and $E_0 \in \mathbb{R}$ a fixed energy, satisfying the following assumptions:

(A1) V_0 is \mathcal{C}^∞ and real-valued on \mathbb{R} .

(A2) There exists $m_0 > 0$ such that, with $\langle x \rangle = (1 + x^2)^{\frac{1}{2}}$,

$$\forall k \in \mathbb{N}, \exists C_k > 0, \forall x \in \mathbb{R}, |V_0^{(k)}(x)| \leq C_k \langle x \rangle^{m_0 - k}.$$

and

$$\forall x \in \mathbb{R} \setminus]-C_0, C_0[, |V_0(x) - E_0| \geq \frac{1}{C_0} \langle x \rangle^{m_0}.$$

(A3) For some $E_0 \in \mathbb{R}$, the equation $V_0(x) = E_0$ has exactly four solutions $\alpha_\ell < \beta_\ell < \beta_r < \alpha_r$, with $V'_0(\alpha_\ell) < 0$, $V'_0(\beta_\ell) > 0$, $V'_0(\beta_r) < 0$, and $V'_0(\alpha_r) > 0$.

Therefore, the operator $P_{h,0}$ on $L^2(\mathbb{R})$ with domain

$$\mathcal{D} = \{u \in H^2(\mathbb{R}), \langle x \rangle^{m_0} u \in L^2(\mathbb{R})\},$$

is a self-adjoint Schrödinger operator with a double-well potential, and its spectrum consists only in real eigenvalues with multiplicity 1.

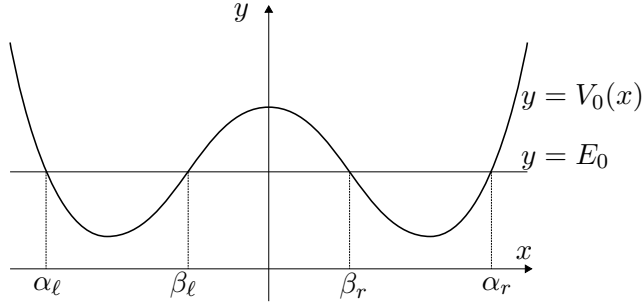


Figure 2: The unperturbed potential V_0

Concerning the perturbation $i\varepsilon W$, we suppose that, with m_0 given in (A2),

(A4) W is a \mathcal{C}^∞ , real-valued function on \mathbb{R} , such that

$$\forall k \in \mathbb{N}, \exists C_k > 0, \forall x \in \mathbb{R}, |W^{(k)}(x)| \leq C_k \langle x \rangle^{m_0-k}.$$

Then, for any $\varepsilon \in]-\varepsilon_0, \varepsilon_0[$ with $\varepsilon_0 > 0$ small enough, the spectrum of the unbounded, closed operator $P_{h,\varepsilon}$ on $L^2(\mathbb{R})$ with domain \mathcal{D} , is still discrete in a complex (h -independent) neighborhood of E_0 . We are interested in the semiclassical asymptotics (i.e. as $h \rightarrow 0$) of the eigenvalues of $P_{h,\varepsilon}$ near E_0 , and we want to know whether they stay real or not for $\varepsilon > 0$ small, under the following \mathcal{PT} -symmetry assumption:

(A5) The operator $P_{h,\varepsilon}$ is \mathcal{PT} -symmetric, that is

$$[P_{h,\varepsilon}, \mathcal{PT}] = 0,$$

where \mathcal{P} is the parity operator, and \mathcal{T} the time-reversal operator given in (1.1).

In terms of the real and imaginary part of the potential V_ε , this assumption is equivalent to the property that V_0 is even and W is odd. In particular, when $\varepsilon = 0$ we have a symmetric double-well potential, and the turning points satisfy

$$(1.3) \quad \alpha_\ell = -\alpha_r, \quad \beta_\ell = -\beta_r.$$

Since we are going to use complex WKB constructions in a neighborhood of the wells, we need to suppose also that

(A6) V_0 and W have analytic extensions to a neighborhood U in \mathbb{C} of the convex hull of $\{x \in \mathbb{R}; V_0(x) \leq E_0\}$.

Remark 1.1 In (A2), and the corresponding assumption on W , we can also treat the case $m_0 = 0$. Then $P_{h,0}$ is still self-adjoint, and its spectrum in $] -\infty, E_0 + 1/C[$ consists also only in eigenvalues. Our results remain valid in this case.

In this paper, we will first obtain a Bohr-Sommerfeld like quantization condition for the eigenvalues of $P_{h,\varepsilon}$ in $D(E_0, 1/C)$. This result does not rely on the \mathcal{PT} -symmetry assumption on $P_{h,\varepsilon}$.

Let us define the relevant action integrals. By the implicit function theorem, there exists $\varepsilon_0 > 0$ such that the equation $V_\varepsilon(z) - E = 0$ has exactly four solutions for $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$, that we denote $\alpha_\ell(E, \varepsilon)$, $\beta_\ell(E, \varepsilon)$, $\beta_r(E, \varepsilon)$ and $\alpha_r(E, \varepsilon)$, depending analytically on E, ε , in such a way that,

$$(1.4) \quad \alpha_\bullet(E_0, 0) = \alpha_\bullet, \quad \beta_\bullet(E_0, 0) = \beta_\bullet, \quad \bullet = \ell, r.$$

These analytic functions of (E, ε) are called turning points at energy E . The action integrals are the functions given by

$$(1.5) \quad I_{\bullet}(E, \varepsilon) = \int_{\alpha_{\bullet}(E, \varepsilon)}^{\beta_{\bullet}(E, \varepsilon)} (E - V_{\varepsilon}(t))^{\frac{1}{2}} dt,$$

where $\bullet = \ell, r$ and the branch of $t \mapsto (E - V_{\varepsilon}(t))^{\frac{1}{2}}$ is the one that is real and positive for $(E, \varepsilon) = (E_0, 0)$ on the segment between α_{\bullet} and β_{\bullet} , $\bullet = \ell, r$, and

$$(1.6) \quad J(E, \varepsilon) = \int_{\beta_l(E, \varepsilon)}^{\beta_r(E, \varepsilon)} (V_{\varepsilon}(t) - E)^{\frac{1}{2}} dt,$$

where $t \mapsto (V_{\varepsilon}(t) - E)^{\frac{1}{2}}$ is real and positive for $(E, \varepsilon) = (E_0, 0)$ on the segment between β_{ℓ} and β_r . These functions I_{ℓ} , I_r and J are analytic with respect to E, ε .

We shall say that a function $f(z, h)$ defined in $\Omega \times]0, h_0]$, analytic with respect to $z \in \Omega$, a domain of \mathbb{C}^d , has an asymptotic expansion

$$f(z, h) \sim \sum_{j \geq 0} f_j(z) h^j$$

in $\text{Hol}(\Omega)$, when the f_j 's are holomorphic in Ω and, for all compact subsets $K \subset \Omega$ and all $N \in \mathbb{N}$,

$$(1.7) \quad \|f(z, h) - \sum_{j=0}^N f_j(z) h^j\|_{L^{\infty}(K)} = \mathcal{O}(h^{N+1}).$$

For a function $k(E, \varepsilon)$ we shall denote, for $\varepsilon \in \mathbb{R}$,

$$(1.8) \quad k^*(E, \varepsilon) = \overline{k(\overline{E}, -\varepsilon)} \quad \text{and} \quad k^{\dagger}(E, \varepsilon) = \overline{k(\overline{E}, \varepsilon)}.$$

Theorem 1.2 *Assume (A1)–(A4) and (A6). There exists a fixed neighborhood $\Omega = \Omega_1 \times \Omega_2$ of $(E_0, 0)$ in $\mathbb{C} \times \mathbb{C}$ and holomorphic functions $\gamma_{\pm}^{\ell}(E, \varepsilon; h)$, $\gamma_{\pm}^r(E, \varepsilon; h)$ with complete asymptotic expansions in $\text{Hol}(\Omega)$ and of the form $1 + \mathcal{O}(h)$ such that if*

$$(1.9) \quad \begin{aligned} f(E, \varepsilon; h) = & \frac{1}{4} \left(e^{iI_{\ell}/h} \gamma_{-}^{\ell} + e^{-iI_{\ell}/h} \gamma_{+}^{\ell} \right) \left(e^{iI_r/h} \gamma_{+}^r + e^{-iI_r/h} \gamma_{-}^r \right) \\ & - \frac{1}{4} e^{-2J/h} \sin(I_{\ell}/h) \sin(I_r/h), \end{aligned}$$

then when $h > 0$ is small enough and $\varepsilon \in \Omega_1 \cap \mathbb{R}$, the eigenvalues of P_ε in Ω_1 coincide with the zeros of $f(\cdot, \varepsilon; h)$ in the same set. The algebraic multiplicity of each such eigenvalue E coincides with the multiplicity of E as a zero of $f(\cdot, \varepsilon; h)$.

We may assume that Ω is invariant under the map $(E, \varepsilon) \mapsto (\overline{E}, \varepsilon)$, and we have

$$(1.10) \quad I_\ell^* = I_\ell, \quad I_r^* = I_r, \quad J^* = J, \quad (\gamma_-^\ell)^* = \gamma_+^\ell, \quad (\gamma_-^r)^* = \gamma_+^r.$$

Assuming also (A5), we have

$$(1.11) \quad f(E, \varepsilon) = \rho \rho^\dagger \cos(\tilde{I}/h) \cos(\tilde{I}^\dagger/h) - \frac{1}{4} e^{-2J/h} \sin(I/h) \sin(I^\dagger/h),$$

where $\rho(E, \varepsilon; h)$, $\tilde{I}(E, \varepsilon; h)$ have complete asymptotic expansions in $\text{Hol}(\Omega)$ with $\rho = 1 + \mathcal{O}(h)$, $\tilde{I} = I + \mathcal{O}(h^2)$. Further, $\tilde{I}^* = \tilde{I}$, $\rho^* = \rho$ and $J^* = J = J^\dagger$.

Remark 1.3 The function f in (1.9) can also be written

$$(1.12) \quad f(E, \varepsilon; h) = \rho_\ell \rho_r \cos(\tilde{I}_\ell/h) \cos(\tilde{I}_r/h) - \frac{1}{4} e^{-2J/h} \sin(I_\ell/h) \sin(I_r/h),$$

where

$$\tilde{I}_\ell - I_\ell, \quad \tilde{I}_r - I_r = \mathcal{O}(h^2), \quad \rho_\ell - 1, \quad \rho_r - 1 = \mathcal{O}(h).$$

These quantities have complete asymptotic expansions in powers of h and enjoy the symmetries,

$$\rho_\ell^* = \rho_\ell, \quad \rho_r^* = \rho_r, \quad \tilde{I}_\ell^* = \tilde{I}_\ell, \quad \tilde{I}_r^* = \tilde{I}_r.$$

Under the additional assumption (A5), we have $\rho_r = \rho_\ell^*$, $\tilde{I}_r = \tilde{I}_\ell^*$ and we get (1.11) with $\rho = \rho_\ell$, $I = I_\ell$, $\tilde{I} = \tilde{I}_\ell$.

The zeros of $E \mapsto \cos(\tilde{I}_\ell/h)$ and $E \mapsto \cos(\tilde{I}_r/h)$ can be thought of as “approximate eigenvalues for the left and right potential wells respectively”. They are given by the Bohr-Sommerfeld quantization conditions,

$$(1.13) \quad 2\tilde{I}_\ell(E, \varepsilon; h) = (2k + 1)\pi h, \quad k \in \mathbb{Z},$$

and

$$(1.14) \quad 2\tilde{I}_r(E, \varepsilon; h) = (2k+1)\pi h, \quad k \in \mathbb{Z},$$

respectively. The last term in (1.12) is exponentially small and represents the tunneling interaction between the potential wells. The solutions $E = \tilde{E}_k^\bullet(\varepsilon; h)$ of (1.13), (1.14) are situated on the curves $\tilde{\Gamma}_\bullet(\varepsilon; h)$ defined by

$$(1.15) \quad \text{Im } \tilde{I}_\bullet(E, \varepsilon; h) = 0,$$

respectively, and the distance between consecutive zeros \tilde{E}_k^\bullet and \tilde{E}_{k+1}^\bullet is of the order h . Here, we use that, for $\bullet = \ell, r$,

$$\partial_E I_\bullet = \frac{1}{2} \int_{\alpha_\bullet}^{\beta_\bullet} (E - V_\varepsilon(x))^{-\frac{1}{2}} dx \neq 0.$$

When $\varepsilon = 0$, $\tilde{\Gamma}_\bullet$ are real neighborhoods of E_0 and the \tilde{E}_k^\bullet are real. We notice that

$$\text{Re } \tilde{E}_k^\ell(\varepsilon) = E_k^\ell(0) + \mathcal{O}(\varepsilon^2).$$

It is clear that the set of zeros of $f(\cdot, \varepsilon; h)$ is (in a suitable sense) exponentially close to the union of the solutions of (1.13) and (1.14). Below we give a such a detailed result in the \mathcal{PT} -symmetric case.

Now we adopt the assumptions (A1)–(A6) as well as the following assumption:

(A7) We have

$$\int_{\alpha_\ell}^{\beta_\ell} (E_0 - V_0(x))^{-\frac{1}{2}} W(x) dx \neq 0.$$

Notice here that

$$2i\partial_\varepsilon I_\ell(E, \varepsilon) = \int_{\alpha_\ell}^{\beta_\ell} (E - V_\varepsilon(x))^{-\frac{1}{2}} W(x) dx.$$

Possibly after the substitution $(\varepsilon, W) \mapsto (-\varepsilon, -W)$, which does not change P_ε , we may assume that the integral in (A7) is > 0 .

Under the assumption (A7), we have $\tilde{I}_\ell^\dagger = \tilde{I}_r$ and hence for real ε , that $\tilde{E}_k^r = \overline{\tilde{E}_k^\ell}$.

Theorem 1.4 *We make the assumptions (A1) to (A7). The values $\tilde{E}_k := \tilde{E}_k^\ell$ and $\tilde{E}_k^r = \overline{\tilde{E}_k}$ are situated on the curves $\tilde{\Gamma} = \tilde{\Gamma}_\ell$ and $\tilde{\Gamma} = \tilde{\Gamma}_r$, where $\tilde{\Gamma}$ is of the form*

$$(1.16) \quad \operatorname{Im} E = \tilde{g}(\operatorname{Re} E, \varepsilon; h).$$

Here

$$(1.17) \quad \tilde{g}(t, \varepsilon; h) \sim g(t, \varepsilon) + hg_1(t, \varepsilon) + \dots \text{ in } \operatorname{Hol}(\operatorname{neigh}(E_0, 0), \mathbb{C}^2)$$

is real for (t, ε) real, and we have,

$$(1.18) \quad \tilde{g}(t, \varepsilon) = \left(\frac{i\partial_\varepsilon I}{\partial_E I}(t, 0) + \mathcal{O}(h^2) \right) \varepsilon + \mathcal{O}(\varepsilon^2).$$

There exists a fixed neighborhood $\Omega = \Omega_1 \times \Omega_2$ of $(E_0, 0) \in \mathbb{C} \times \mathbb{R}$, such that for $\varepsilon \in \Omega_2$ and for $h > 0$ small enough,

$$(1.19) \quad f^{-1}(0, \varepsilon) \subset \bigcup_k D\left(\tilde{E}_k, r(\tilde{E}_k, \varepsilon)\right) \cup \bigcup_k D\left(\overline{\tilde{E}_k}, r\left(\overline{\tilde{E}_k}, \varepsilon\right)\right),$$

where $r(E, \varepsilon) \leq Ch e^{-\operatorname{Re} J(E, \varepsilon)/h}$ is given by

$$(1.20) \quad r(E, \varepsilon) = Ch \min\left(1, \max(h/\varepsilon, 1)e^{-\operatorname{Re} J(E, \varepsilon)/h}\right) e^{-\operatorname{Re} J(E, \varepsilon)/h}.$$

and $C > 0$ is large enough. Moreover,

- when these discs are disjoint, $f(\cdot, \varepsilon)$ has precisely one zero in each of $D\left(\tilde{E}_k, r\left(\tilde{E}_k, \varepsilon\right)\right)$ and $D\left(\overline{\tilde{E}_k}, r\left(\overline{\tilde{E}_k}, \varepsilon\right)\right)$.
- in general $f(\cdot, \varepsilon)$ has precisely 2 zeros in

$$D\left(\tilde{E}_k, r\left(\tilde{E}_k, \varepsilon\right)\right) \cup D\left(\overline{\tilde{E}_k}, r\left(\overline{\tilde{E}_k}, \varepsilon\right)\right).$$

We finally discuss the more precise behaviour of the eigenvalues when $|\varepsilon|$ is exponentially small. The function

$$f/(\rho\rho^\dagger) = \cos\left(\frac{\tilde{I}}{h}\right) \cos\left(\frac{\tilde{I}^\dagger}{h}\right) - \frac{1}{4\rho\rho^\dagger} e^{-2J/h} \sin\left(\frac{I}{h}\right) \sin\left(\frac{I^\dagger}{h}\right),$$

is real-valued on the real axis and has a sequence of local minima $E_k(\varepsilon; h)$ such that

$$E_k(0; h) = E_k^\ell(0; h) + \mathcal{O}\left(he^{-2J(E_k^\ell(0; h), 0)/h}\right),$$

where $E_k^\ell(0; h) = E_k^r(0; h)$ is defined in (1.13), (1.14) and we know that when $|\varepsilon| \leq e^{-1/(Ch)}$, there are two eigenvalues of P_ε exponentially close to $E_k(0; h)$ and that we obtain in this way all the eigenvalues in a fixed neighborhood of E_0 . It will be convenient to introduce a “Floquet parameter” $\kappa \in \mathbb{R}$ and to set

$$\begin{aligned} \tilde{f}(E, \varepsilon, \kappa; h) = \\ \cos\left(\frac{\tilde{I}}{h} - \kappa\right) \cos\left(\frac{\tilde{I}^\dagger}{h} - \kappa\right) - \frac{e^{-2J/h}}{4\rho\rho^\dagger} \sin\left(\frac{I}{h} - \kappa\right) \sin\left(\frac{I^\dagger}{h} - \kappa\right). \end{aligned}$$

We still have a sequence of local minima $E_k(\varepsilon, \kappa; h)$ satisfying $E_k(\varepsilon, \kappa + \pi; h) = E_{k+1}(\varepsilon, \kappa; h)$ and the zeros of $\tilde{f}(\cdot, \varepsilon, \kappa; h)$ are now confined, two by two, to exponentially small neighborhoods of $E_k(\varepsilon, \kappa; h)$. We concentrate on one such local minimum $E_c(\varepsilon, \kappa; h) = E_k(\varepsilon, \kappa; h)$ and we restrict the attention to a “window”

$$(1.21) \quad E = E_1 + hF, \quad \varepsilon = h\tilde{\varepsilon}, \quad \kappa = \tilde{\kappa} + I(E_1, 0)/h,$$

where E_1 is a real parameter $\in \text{neigh}(E_0, \mathbb{R})$. Assume that $E_c(\varepsilon, \kappa; h)$ belongs to the window, so that

$$(1.22) \quad E_c(\varepsilon, \kappa; h) = E_1 + hF_c(\tilde{\varepsilon}, \tilde{\kappa}; h),$$

where F_c is the corresponding critical point of \tilde{f} in the variables F with $\tilde{\varepsilon}, \tilde{\kappa}$ as the new parameters. Thanks to the rescaling, this critical point is uniformly nondegenerate. \tilde{f} and F_c are even functions of $\tilde{\varepsilon}$ and it follows that

$$(1.23) \quad F_c(\tilde{\varepsilon}, \tilde{\kappa}; h) = F_c(0, \tilde{\kappa}; h) + \mathcal{O}(\tilde{\varepsilon}^2).$$

We make the assumptions (A1)–(A7) and discuss the zeros of \tilde{f} near the critical value $E_c(\varepsilon, \kappa; h) = E_1 + hF_c(\tilde{\varepsilon}, \tilde{\kappa}; h)$. The key point is that, in this regime, we are able to write the quantization condition as a second order polynomial (up to a non-vanishing factor), with a sharp control on the coefficients.

Theorem 1.5 *The critical value $\tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) = \tilde{f}(F_c, \tilde{\varepsilon}, \tilde{\kappa}; h)$ is of the form*

$$(1.24) \quad \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) = m(\tilde{\varepsilon}, \tilde{\kappa}; h)(\tilde{\varepsilon}^2 - \tilde{\varepsilon}_c(\tilde{\kappa}; h)^2),$$

where

$$(1.25) \quad \tilde{\varepsilon}_c = \ell(\tilde{\kappa}; h)e^{-J(E_c(0, \kappa), 1)/h}.$$

Here, ℓ , m are classical symbols of order 0 as in (1.7), with leading terms satisfying

$$(1.26) \quad \ell(\tilde{\kappa}; 0) = \frac{1}{2|\partial_{\varepsilon}I(E_1, 0)|}, \quad m(0, \tilde{\kappa}; 0) = |\partial_{\varepsilon}I(E_1, 0)|.$$

Further,

$$(1.27) \quad \tilde{f}(F, \tilde{\varepsilon}, \tilde{\kappa}; h) = \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) + q(F, \tilde{\varepsilon}, \tilde{\kappa}; h)(F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h))^2,$$

where q is a symbol of order 0 and

$$(1.28) \quad q(F_c, 0, \tilde{\kappa}; 0) = 2(\partial_E \tilde{I}(E_c(0, \kappa, 0), 0))^2.$$

$\tilde{f}(\cdot, \tilde{\varepsilon}, \tilde{\kappa}; h)$ has two zeros in a small neighborhood of F_c when counted with their multiplicity, and

- when $|\tilde{\varepsilon}| < \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ the zeros are real and simple, given by

$$(1.29) \quad q(F, \tilde{\varepsilon}, \tilde{\kappa}; h)^{\frac{1}{2}}(F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h)) = \pm(-\tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h))^{\frac{1}{2}}$$

- when $|\tilde{\varepsilon}| = \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ we have a double zero,

$$(1.30) \quad F = F_c.$$

- when $|\tilde{\varepsilon}| > \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ the zeros are simple, non-real and complex conjugate to each other, given by

$$(1.31) \quad q(F, \tilde{\varepsilon}, \tilde{\kappa}; h)^{\frac{1}{2}}(F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h)) = \pm i(\tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h))^{\frac{1}{2}}.$$

When $\kappa = \tilde{\kappa} + I(E_1, 0)/h$ belongs to $\pi\mathbb{Z}$, these values give the eigenvalues of P_{ε} near $E_c(\varepsilon, \kappa; h)$ via (1.21).

Eventually, we would like to mention the paper [13] by C. Gérard and A. Grigis, where the authors study the eigenvalues of self-adjoint Schrödinger operators with a double well potential. They also obtain a quantization condition, using what they call the "exact WKB method". Our method here is slightly different and more explicit about the connection formulas at the turning points.

2 The complex WKB method

We recall here briefly elements of the complex WKB method in a general setting. Consider a Schrödinger equation,

$$(2.1) \quad -h^2 u''(z, h) + V(z)u(z, h) = 0,$$

in a bounded, simply connected open set $U \subset \mathbb{C}$ where the potential V is holomorphic. We look for a solution of the type

$$(2.2) \quad u(z, h) = a(z, h)e^{i\varphi(z)/h},$$

where $a(z, h)$ has a formal asymptotic expansion in a sense to be defined later on,

$$(2.3) \quad a(z, h) \sim \sum_{j=0}^{+\infty} a_j(z)h^j,$$

and the a_j 's are holomorphic functions in U . The function φ is called the phase of the solution u , and $a(z, h)$ is called its symbol.

A function $u(z, h)$ of the form (2.2) is a solution to (2.1) if and only if

$$(2.4) \quad e^{-i\varphi(z)/h}(-h^2 \partial_z^2 + V(z))(e^{i\varphi(z)/h}a(z, h)) = 0,$$

or

$$(2.5) \quad (-(h\partial_z)^2 - 2i\varphi'(z)h\partial_z - ih\varphi''(z) + \varphi'(z)^2 + V(z))a(z, h) = 0.$$

If φ is a solution of the eikonal equation

$$(2.6) \quad \varphi'(z)^2 + V(z) = 0,$$

then (2.4) is equivalent to

$$(2.7) \quad \left(\varphi'(z)\partial_z + \frac{\varphi''(z)}{2} - \frac{ih}{2}\partial_z^2 \right) a(z, h) = 0.$$

Replacing $a(z, h)$ by its formal asymptotic expansion (2.3), and canceling successively the powers of h , we obtain a sequence of transport equations

$$(2.8) \quad \begin{cases} \left(\varphi'(z)\partial_z + \frac{1}{2}\varphi''(z) \right) a_0 = 0, \\ \left(\varphi'(z)\partial_z + \frac{1}{2}\varphi''(z) \right) a_j = \frac{i}{2}a''_{j-1}, \text{ for } j \geq 1. \end{cases}$$

Definition 2.1 A formal WKB solution u_{wkb} of the equation (2.1) in U is a pair $(\varphi, (a_j))$ of an analytic function φ in U verifying the eikonal equation (2.6), and of a sequence (a_j) of analytic functions in U which satisfies the transport equations (2.8). We denote it

$$(2.9) \quad u_{wkb}(z, h) = e^{i\varphi(z)/h} \sum_{j \geq 0} a_j(z) h^j.$$

We suppose from now on that $V(z) \neq 0$ for all $z \in U$. Then we fix a determination of $z \mapsto (-V(z))^{\frac{1}{2}}$ in U , and we solve the eikonal and transport equations in U .

Proposition 2.2 The solutions of the eikonal equation (2.6) are analytic functions in U , and they can be written

$$(2.10) \quad \varphi(z) = \pm \int_{z_0}^z (-V(w))^{\frac{1}{2}} dw + C$$

for some $z_0 \in U$, and some $C \in \mathbb{C}$.

Now we fix a such a solution φ in U . It is then easy to prove by induction that, given an initial data, the system of transport equations has a unique solution. Therefore we have the

Proposition 2.3 Let $(a_j^0)_{j=0}^\infty$ be any sequence of complex numbers. Then the Schrödinger equation (2.1) has a unique formal WKB solution in U , such that

$$\forall j \in \mathbb{N}, a_j(z_0) = a_j^0.$$

Moreover, the function a_0 is given in U , for some suitable constant $C \in \mathbb{C}$, by

$$a_0(z) = C(\varphi'(z))^{-1/2}.$$

We want now to associate true solutions of the Schrödinger equation (2.1) to the formal ones we have constructed above. It is convenient to introduce the notion of Stokes line for the potential V .

Definition 2.4 Let U be a simply connected open set in \mathbb{C} where V is holomorphic. A Stokes line is a C^1 curve $\sigma : I \rightarrow U$ such that

$$\operatorname{Im} \int_s^t (-V(\sigma(\tau)))^{\frac{1}{2}} \sigma'(\tau) d\tau = 0,$$

for all $s, t \in I$. Here, I is any interval starting at 0 and ending at 1.

Notice that

$$\operatorname{Im} \int_s^t (-V(\sigma(\tau)))^{\frac{1}{2}} \sigma'(\tau) d\tau = \operatorname{Im}(\varphi(\sigma(t))) - \operatorname{Im}(\varphi(\sigma(s))),$$

where φ is a solution of the eikonal equation. Thus, a Stokes line is nothing else than a level curve in U of the imaginary part of the phase φ .

The following proposition is well known (see for example [23] for a proof), and can be considered as the fundamental rule of the complex WKB method: always move in a direction where the modulus of the phase factor increases, thus in particular transversely to the Stokes lines.

Proposition 2.5 Let U be a simply connected bounded open subset of \mathbb{C} , such that $V(z) \neq 0$ for all $z \in U$. Let φ be a solution of the eikonal equation in U . Let also $\gamma :]0, 1[\rightarrow U$ be a C^1 curve in U such that

$$(2.11) \quad \forall t \in]0, 1[, \quad \frac{d}{dt}(-\operatorname{Im} \varphi(\gamma(t))) > 0,$$

Then there exists a neighborhood $\Omega \subset U$ of γ such that, for any formal WKB solution $u_{wkb}(z, h) = e^{i\varphi(z)/h} \sum_{j \geq 0} a_j(z) h^j$, there exists a solution u of the Schrödinger equation (2.1) in Ω such that

$$(2.12) \quad u(z, h) = e^{i\varphi(z)/h} a(z, h),$$

where a is holomorphic with respect to $z \in \Omega$, and

$$(2.13) \quad a(z, h) \sim \sum_{k \geq 0} a_k(z) h^k \text{ in } \operatorname{Hol}(\Omega).$$

3 WKB analysis near a simple turning point

In this section we follow closely the presentation in [23]. Let $\Omega \subset \mathbb{C}$ be open and simply connected, and $V \in \text{Hol}(\Omega)$. We suppose that V has a unique zero z_0 in Ω , and that it is a simple one:

$$(3.1) \quad V(z_0) = 0, \quad V'(z_0) \neq 0.$$

We are interested in solutions u in Ω of the general Schrödinger equation (2.1) of the form

$$(3.2) \quad u(z, h) = a(z, h)e^{\varphi(z)/h}.$$

Notice that, contrary to (2.2), here we have chosen not to put the factor i in the exponent to simplify the notations. For the same reason, we will also assume that $z_0 = 0$.

As in Section 2, we obtain first the eikonal equation

$$(3.3) \quad \varphi'(z) = V(z)^{\frac{1}{2}},$$

in Ω . By assumption there exists a function F , holomorphic in Ω , such that

$$V(z) = zF(z)$$

and $F(z) \neq 0$ for $z \in \Omega$ (we may decrease Ω whenever necessary). It is therefore clear that $\varphi(z)$ is multi-valued in general, and to better understand the structure of this singularity we pass to the double covering $\tilde{\Omega}$ of $\Omega \setminus \{0\}$, setting $z = w^2$. Then

$$\frac{\partial}{\partial z} = \frac{1}{2w} \frac{\partial}{\partial w},$$

and if we set

$$\begin{cases} \tilde{V}(w) = V(z) = w^2 F(w^2), \\ \tilde{\varphi}(w) = \varphi(z), \end{cases}$$

the eikonal equation becomes

$$\partial_w \tilde{\varphi}(w) = 2w^2 F(w^2)^{\frac{1}{2}}.$$

Notice that the right hand side is an even holomorphic function. If we also require that $\varphi(0) = \tilde{\varphi}(0) = 0$, we see that $\tilde{\varphi}(w)$ is an odd holomorphic function of the form

$$\tilde{\varphi}(w) = \frac{2}{3} \tilde{F}(w^2) w^3, \quad \text{where } \tilde{F}(0) = F(0)^{\frac{1}{2}} = V'(0)^{\frac{1}{2}}.$$

In the original coordinates, we get the double-valued solution,

$$(3.4) \quad \varphi(z) = \frac{2}{3} \tilde{F}(z) z^{\frac{3}{2}}.$$

Now we study the Stokes and anti-Stokes lines having 0 as a limit point. Since, with respect to Section 2, we have removed the factor i in the exponent in (3.2), Stokes lines are now level curves of the real part of φ , and level curves of $\text{Im } \varphi$ are called anti-Stokes lines. On such curves we have $\text{Re } \varphi = 0$ or $\text{Im } \varphi = 0$, which is equivalent to $\text{Im } \varphi^2 = 0$, and to $\text{Im } z^3 \tilde{F}(z)^2 = 0$. In other words, these curves are given by

$$(3.5) \quad \{z \in \Omega, \exists t \in \mathbb{R}, z^3 \tilde{F}(z)^2 = t^3\}.$$

Taking the cubic root, we see that Stokes and anti-Stokes lines reaching 0 in the limit, are contained in three curves γ_k given by

$$(3.6) \quad \gamma_k = \{z \in \Omega, \exists t \in \mathbb{R}, z \tilde{F}(z)^{\frac{2}{3}} = e^{2\pi i k/3} t\}, \quad k \in \{0, 1, 2\} \simeq \mathbb{Z}/3\mathbb{Z}.$$

In the case where $V'(0) > 0$, the situation is as shown in Figure 3. Each curve $\gamma_k \setminus \{0\}$ is divided into a Stokes line γ_k^- (plain lines) and an anti-Stokes line γ_k^+ (dashed lines). The three Stokes lines delimit three closed Stokes sectors Σ_k , $k \in \mathbb{Z}/3\mathbb{Z}$, where Σ_k is the sector that contains γ_k^+ . In Figure 3, we have also drawn a Stokes line inside each sector.

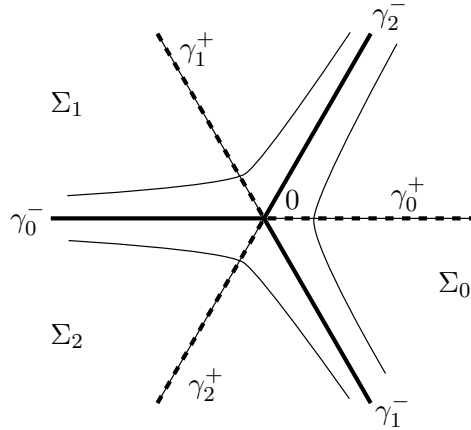


Figure 3: Stokes lines close to a simple turning point

For $k \in \mathbb{Z}/3\mathbb{Z}$, we denote by φ_k the branch of φ in $\Omega \setminus \gamma_k^-$ such that $\varphi_k(0) = 0$, and $\text{Re } \varphi_k < 0$ in Σ_k . Notice that φ_{k+1} and φ_k are both well

defined in $\Sigma_k \cup \Sigma_{k+1}$ and satisfy

$$(3.7) \quad \varphi_{k+1} = -\varphi_k \text{ in } \Sigma_k \cup \Sigma_{k+1}.$$

According to Proposition 2.5, there are solutions $u = u_k$, $k \in \mathbb{Z}/3\mathbb{Z}$, of the Schrödinger equation (2.1) in Ω such that, in $\mathring{\Sigma}_k$,

$$(3.8) \quad \begin{cases} u_k(z, h) = a_k(z, h)e^{\varphi_k(z)/h}, \\ a_k(z, h) \sim \sum_{j \geq 0} a_{k,j}(z)h^j \text{ in } \text{Hol}(\mathring{\Sigma}_k). \end{cases}$$

This asymptotic description extends to Ω_k , the complement of an arbitrarily small neighborhood of $\gamma_k^- \cup \{0\}$, that can be reached from Σ_k by crossing the Stokes lines transversally. We also recall that $a_{k,0}$ is unique up to a constant factor and that we can choose

$$(3.9) \quad a_{k,0}(z) = (\varphi'_k(z))^{-\frac{1}{2}},$$

for any branch of the square root.

Recall that if u, v are solutions to the Schrödinger equation, then the Wronskian

$$W_h(u, v) = (h\partial_z u)v - u(h\partial_z v).$$

is constant, and vanishes precisely when u, v are collinear. Let $j, k \in \mathbb{Z}/3\mathbb{Z}$. Applying the asymptotics of u_j and u_k at some point in the interior of $\Sigma_j \cup \Sigma_k$, we see that, recalling (3.9), $W_h(u_j, u_k)$ has an asymptotic expansion in powers of h , whose first term is given by

$$(3.10) \quad W_h(u_j, u_k) = 2a_{j,0}a_{k,0}\varphi'_j + \mathcal{O}(h) = \frac{2(\varphi'_j)^{\frac{1}{2}}}{(\varphi'_k)^{\frac{1}{2}}} + \mathcal{O}(h).$$

We fix a branch of $(\varphi'_k)^{\frac{1}{2}}$ in Σ_k for each $k \in \mathbb{Z}/3\mathbb{Z}$. For two different Stokes sectors, $\Sigma_j \neq \Sigma_k$, we have in the interior of $\Sigma_j \cup \Sigma_k$, that

$$(3.11) \quad (\varphi'_j)^{\frac{1}{2}} = i^{\nu_{j,k}}(\varphi'_k)^{\frac{1}{2}},$$

for some $\nu_{j,k} \in \mathbb{Z}/4\mathbb{Z}$ which are odd, and such that $\nu_{j,k} = -\nu_{k,j}$. Thus, starting from Σ_0 , we can make a tour around 0 in the positive direction and we get that

$$(3.12) \quad \begin{aligned} (\varphi'_1)^{\frac{1}{2}} &= i^{\nu_{1,0}}(\varphi'_0)^{\frac{1}{2}} \text{ in } \Sigma_1, \\ (\varphi'_2)^{\frac{1}{2}} &= i^{\nu_{2,1}}(\varphi'_1)^{\frac{1}{2}} \text{ in } \Sigma_2, \\ (\varphi'_0)^{\frac{1}{2}} &= i^{\nu_{0,2}}(\varphi'_2)^{\frac{1}{2}} \text{ in } \Sigma_0. \end{aligned}$$

This means that if we follow a continuous branch of $(\varphi'_0)^{\frac{1}{2}}$ around 0 in the positive direction, then after a turn, we obtain the new branch

$$(3.13) \quad i^{-(\nu_{0,2}+\nu_{2,1}+\nu_{1,0})}(\varphi'_0)^{\frac{1}{2}}.$$

But $(\varphi'_0)^{\frac{1}{2}} = V^{1/4}$ for a suitable branch of the fourth root, and if one follows this function around 0 once in the positive direction, we obtain $iV^{1/4}$. This gives the co-cycle condition

$$(3.14) \quad \nu_{0,2} + \nu_{2,1} + \nu_{1,0} \equiv -1 \pmod{4}.$$

(3.10) and (3.11) imply that

$$W_h(u_j, u_k) = 2i^{\nu_{j,k}} + \mathcal{O}(h).$$

Now we describe the linear space of solutions of the Schrödinger equation (2.1) in Ω . It is of course of dimension 2, and any two of u_{-1} , u_0 , u_1 are linearly independent, so we have a relation

$$(3.15) \quad \alpha_{-1}u_{-1} + \alpha_0u_0 + \alpha_1u_1 = 0,$$

where the vector $(\alpha_{-1}, \alpha_0, \alpha_1)^T \in \mathbb{C}^3 \setminus \{0\}$ is well defined up to a scalar factor. Applying $W(u_j, \cdot)$ to this relation, we get

$$(3.16) \quad (W(u_j, u_k))_{j,k} \begin{pmatrix} \alpha_{-1} \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = 0,$$

which is a system of the form

$$(3.17) \quad \begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix} \begin{pmatrix} \alpha_{-1} \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = 0.$$

The triplet $(\alpha_{-1}, \alpha_0, \alpha_1) = (c, -b, a)$ is a solution, so up to a common factor, we have

$$(3.18) \quad \alpha_j = \pm i + \mathcal{O}(h).$$

More precisely, the values of a, b and c are given by the equation (3.15), and we get, after inserting a factor $1/2$,

$$(3.19) \quad \begin{pmatrix} \alpha_{-1} \\ \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} i^{\nu_{0,1}} \\ -i^{\nu_{-1,1}} \\ i^{\nu_{-1,0}} \end{pmatrix} + \mathcal{O}(h) = \begin{pmatrix} i^{\nu_{0,1}} \\ i^{\nu_{1,-1}} \\ i^{\nu_{-1,0}} \end{pmatrix} + \mathcal{O}(h).$$

Remark 3.1 Sometimes it is more natural to change the notation, writing $i\varphi_j$ in (3.8) instead of φ_j so that $u_j(z; h) = a_j(z; h)e^{i\varphi_j(z)/h}$ with $\text{Im } \varphi_j \geq 0$ in Σ_j . Then (3.9) becomes $a_{j,0}(z) = (i\varphi'_j)^{-1/2} = V(z)^{-1/4}$ and in (3.11), (3.12), φ'_j must be replaced by $i\varphi'_j$.

4 WKB solutions near the wells

From now on, we consider the equation $P_{h,\varepsilon}u = Eu$, that is

$$(4.1) \quad -h^2 u'' + (V_\varepsilon(x) - E)u = 0,$$

where $V_\varepsilon = V_0 + i\varepsilon W$ satisfies (A1) to (A4) and (A6). For the moment we do not assume the \mathcal{PT} -symmetry property (A5).

Let us now define some formal WKB solutions to the Schrödinger equation (4.1) near the wells. For $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$, the equation $V_\varepsilon(x) = E$ has exactly four solutions in U , the domain of holomorphy of V_ε , that are called turning points at energy E . We have denoted them $\alpha_\ell(E, \varepsilon)$, $\beta_\ell(E, \varepsilon)$, $\beta_r(E, \varepsilon)$ and $\alpha_r(E, \varepsilon)$, with,

$$(4.2) \quad \alpha_\bullet(E_0, 0) = \alpha_\bullet, \quad \beta_\bullet(E_0, 0) = \beta_\bullet, \quad \bullet = \ell, r.$$

We have drawn in Figure 4 a typical configuration of the Stokes lines starting at each of the turning points, when $E \neq E_0$ and $\varepsilon \neq 0$.

We shall work in the cut complex plane along $[\alpha_\ell, \beta_\ell] \cup [\beta_r, \alpha_r]$, or more precisely in the cut version \tilde{U} of U , so that we have two determinations of $x \mapsto (V_\varepsilon(x) - E)^{\frac{1}{2}}$ in \tilde{U} . We denote

$$x \mapsto (V_\varepsilon(x) - E)_\ell^{\frac{1}{2}}, \text{ (resp. } x \mapsto (V_\varepsilon(x) - E)_m^{\frac{1}{2}}, \text{ } x \mapsto (V_\varepsilon(x) - E)_r^{\frac{1}{2}}),$$

the determination which is real and positive for $\varepsilon = 0$, $E = E_0$ and $x \in]-\infty, \alpha_\ell[$ (resp. $x \in]\beta_\ell, \beta_r[$, $x \in]\alpha_r, +\infty[$). Notice that

$$\forall x \in \tilde{U}, \quad (V_\varepsilon(x) - E)_\ell^{\frac{1}{2}} = (V_\varepsilon(x) - E)_r^{\frac{1}{2}} = -(V_\varepsilon(x) - E)_m^{\frac{1}{2}}.$$

First, we concentrate on the situation near the left well. We denote Σ_0^ℓ , Σ_1^ℓ and Σ_{-1}^ℓ the three Stokes sectors near α_ℓ , and S_0^ℓ , S_1^ℓ and S_{-1}^ℓ those near

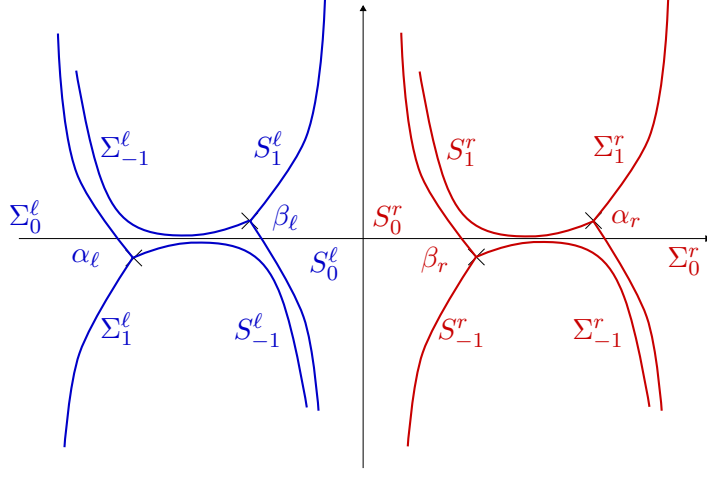


Figure 4: Stokes lines and Stokes sectors

β_ℓ . For each sector Σ_k^ℓ (resp. S_k^ℓ), $k \in \mathbb{Z}/3\mathbb{Z}$, we choose a solution u_k^ℓ (resp. v_k^ℓ) of (4.1) such that

$$(4.3) \quad \begin{aligned} u_k^\ell(z, E, \varepsilon, h) &= a_k^\ell(z, E, \varepsilon, h) e^{i\varphi_k^\ell(z, E, \varepsilon)/h} \text{ in } \Sigma_k^\ell \\ v_k^\ell(z, E, \varepsilon, h) &= b_k^\ell(z, E, \varepsilon, h) e^{i\psi_k^\ell(z, E, \varepsilon)/h} \text{ in } S_k^\ell. \end{aligned}$$

Here φ_k^ℓ (resp. ψ_k^ℓ) is a solution of the eikonal equation

$$(4.4) \quad (i\varphi'(x))^2 = V_\varepsilon(x) - E,$$

vanishing at $z = \alpha_\ell(E, \varepsilon)$ (resp. at $\beta_\ell(E, \varepsilon)$) for $(E, \varepsilon) \in D(E_0, \varepsilon) \times D(0, \varepsilon_0)$, such that

$$(4.5) \quad \begin{aligned} \forall z \in \Sigma_k^\ell, \operatorname{Re}(i\varphi_k^\ell(z, E, \varepsilon)) &< 0, \\ \forall z \in S_k^\ell, \operatorname{Re}(i\psi_k^\ell(z, E, \varepsilon)) &< 0. \end{aligned}$$

The amplitudes a_k^ℓ and b_k^ℓ in (4.3) have asymptotic expansions in $\operatorname{Hol}(\mathring{\Sigma}_k^\ell)$ and $\operatorname{Hol}(\mathring{S}_k^\ell)$ respectively, in the sense of (1.7). The phase functions φ_k^ℓ and φ_{k+1}^ℓ are well defined in $\Sigma_k^\ell \cup \Sigma_{k+1}^\ell$, and $\psi_k^\ell, \psi_{k+1}^\ell$ are well defined in $S_k^\ell \cup S_{k+1}^\ell$, where they satisfy

$$(4.6) \quad \varphi_k^\ell = -\varphi_{k+1}^\ell, \quad \psi_k^\ell = -\psi_{k+1}^\ell.$$

We choose the functions u_k^ℓ (resp. v_k^ℓ) so that they are holomorphic also with respect to (E, ε) in $D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$. The asymptotic expansions

of the amplitudes a_k^ℓ and b_k^ℓ extend to $\Omega_k^\ell \times D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$ and $\mathcal{O}_k^\ell \times D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$ respectively, where Ω_k^ℓ (resp. \mathcal{O}_k^ℓ) is the complement of an arbitrarily small neighborhood of $\gamma_{\alpha_\ell, k}^-$ (resp. $\gamma_{\beta_\ell, k}^-$) in U (see Figure 3).

We fix now a choice for the principal symbols $a_{k,0}^\ell$ and $b_{k,0}^\ell$ of these six solutions u_k^ℓ and v_k^ℓ , $k \in \mathbb{Z}/3\mathbb{Z}$.

By (4.4) and (4.5) we have

$$(4.7) \quad \begin{cases} i\varphi_0^\ell(x, E, \varepsilon) = \int_{\alpha_\ell}^x (V_\varepsilon(t) - E)_\ell^{\frac{1}{2}} dt, \\ i\varphi_{-1}^\ell(x, E, \varepsilon) = - \int_{\alpha_\ell}^x (V_\varepsilon(t) - E)_\ell^{\frac{1}{2}} dt, \\ i\varphi_1^\ell(x, E, \varepsilon) = - \int_{\alpha_\ell}^x (V_\varepsilon(t) - E)_\ell^{\frac{1}{2}} dt. \end{cases}$$

Then we choose the principal symbol $a_{0,0}^\ell$ of a_0^ℓ to be

$$(4.8) \quad a_{0,0}^\ell(x, E, \varepsilon) = [(i\varphi_0^\ell)']^{-\frac{1}{2}} = (V_\varepsilon(x) - E)_\ell^{-\frac{1}{4}}.$$

In order to fix the principal symbol of u_1^ℓ and u_{-1}^ℓ , we have to choose $\nu_{0,1}, \nu_{1,-1}$ and $\nu_{-1,0}$ in $\mathbb{Z}/4\mathbb{Z}$, odd, such that (3.14) holds. We take

$$(4.9) \quad \nu_{0,1} = 1, \nu_{1,-1} = -1, \text{ and } \nu_{-1,0} = 1.$$

Then by (3.12) we have,

$$(4.10) \quad a_{-1,0}^\ell(x, E, \varepsilon) = \frac{1}{i^{\nu_{-1,0}}} a_{0,0}^\ell(x, E, \varepsilon) = -i(V_\varepsilon(x) - E)_\ell^{-\frac{1}{4}},$$

and,

$$(4.11) \quad a_{1,0}^\ell(x, E, \varepsilon) = \frac{1}{i^{\nu_{1,0}}} a_{0,0}^\ell(x, E, \varepsilon) = i(V_\varepsilon(x) - E)_\ell^{-\frac{1}{4}}.$$

With these choices, we have

$$(4.12) \quad u_0^\ell = \tau_+(h)u_{-1}^\ell + \tau_-(h)u_1^\ell,$$

for some symbols $\tau_\pm(h)$ with $\tau_\pm(h) = 1 + \mathcal{O}(h)$. Without changing the leading asymptotics, we can replace $u_{\mp 1}^\ell$ by $\tau_\pm^\ell u_{\mp 1}^\ell$ and we get

$$(4.13) \quad u_0^\ell = u_{-1}^\ell + u_1^\ell.$$

Let us now consider the solutions v_k^ℓ , $k \in \mathbb{Z}/3\mathbb{Z}$, near β_ℓ . By (4.4) and (4.5) we have

$$(4.14) \quad \begin{cases} i\psi_0^\ell(x, E, \varepsilon) = - \int_{\beta_\ell}^x (V_\varepsilon(t) - E)_m^{\frac{1}{2}} dt, \\ i\psi_{-1}^\ell(x, E, \varepsilon) = \int_{\beta_\ell}^x (V_\varepsilon(t) - E)_m^{\frac{1}{2}} dt, \\ i\psi_1^\ell(x, E, \varepsilon) = \int_{\beta_\ell}^x (V_\varepsilon(t) - E)_m^{\frac{1}{2}} dt. \end{cases}$$

We here consider $-z$ as the basic variable for the Schrödinger equation and correspondingly, we choose the principal symbol $b_{0,0}^\ell$ of b_0^ℓ to be

$$(4.15) \quad b_{0,0}^\ell(x, E, \varepsilon) = [(-i\psi_0^\ell)']^{-\frac{1}{2}} = (V_\varepsilon(x) - E)_m^{-\frac{1}{4}},$$

and we fix the principal symbol of v_1^ℓ and v_{-1}^ℓ , choosing $\nu_{0,1}, \nu_{1,-1}$ and $\nu_{-1,0}$ as in (4.9):

$$(4.16) \quad \nu_{0,1} = 1, \quad \nu_{1,-1} = -1, \quad \text{and} \quad \nu_{-1,0} = 1.$$

We get,

$$(4.17) \quad b_{-1,0}^\ell(x, E, \varepsilon) = \frac{1}{i^{\nu_{-1,0}}} b_{0,0}^\ell(x, E, \varepsilon) = -i(V_\varepsilon(x) - E)_m^{-\frac{1}{4}},$$

and

$$(4.18) \quad b_{1,0}^\ell(x, E, \varepsilon) = \frac{1}{i^{\nu_{1,0}}} b_{0,0}^\ell(x, E, \varepsilon) = i(V_\varepsilon(x) - E)_m^{-\frac{1}{4}}.$$

We further fix a choice of $v_{\pm 1}^\ell$. The principle of the WKB method ensures that we can choose v_1^ℓ to be proportional to u_{-1}^ℓ , and v_{-1}^ℓ to be proportional to u_1^ℓ . Notice first that

$$i\psi_1^\ell(x, E, \varepsilon) - i\varphi_{-1}^\ell(x, E, \varepsilon) = \int_{\alpha_\ell}^{\beta_\ell} (V_\varepsilon(t) - E)_\ell^{\frac{1}{2}} dt = -iI_\ell(E, h),$$

where we have set

$$(4.19) \quad I_\ell(E, \varepsilon) = \int_{\alpha_\ell}^{\beta_\ell} (E - V_\varepsilon(t))_w^{\frac{1}{2}} dt$$

where $(E - V_\varepsilon(t))^{\frac{1}{2}}$ is real and positive for $\varepsilon = 0$, $E \in \mathbb{R}$ close to E_0 and $t \in]\alpha_\ell, \beta_\ell[$. The same way, we see that

$$i\psi_{-1}^\ell(x, E, \varepsilon) - i\varphi_1^\ell(x, E, \varepsilon) = iI_\ell(E, h).$$

Concerning the principal symbols, we have first

$$(4.20) \quad \begin{aligned} (V_\varepsilon(x) - E)_{\ell+}^{\frac{1}{4}} &= -i(V_\varepsilon(x) - E)_m^{\frac{1}{4}}, \\ (V_\varepsilon(x) - E)_{\ell-}^{\frac{1}{4}} &= i(V_\varepsilon(x) - E)_m^{\frac{1}{4}}. \end{aligned}$$

Here we have denoted $(V_\varepsilon(x) - E)_{l+}^{-\frac{1}{4}}$ (resp. $(V_\varepsilon(x) - E)_{l-}^{-\frac{1}{4}}$) the determination of $(V_\varepsilon(x) - E)^{-\frac{1}{4}}$ obtained on $] \beta_\ell, \beta_r[$ by extending $(V_\varepsilon(x) - E)_\ell^{-\frac{1}{4}}$ on \tilde{U} along a path in the upper (resp. lower) half plane. Thus we see that

$$(4.21) \quad b_{1,0}^\ell = ia_{-1,0}^\ell \quad \text{and} \quad b_{-1,0}^\ell = -ia_{1,0}^\ell,$$

and we can assume that

$$\begin{cases} u_{-1}^\ell = -ie^{iI_\ell(E, \varepsilon)/h} \sigma_+^\ell v_1^\ell, \\ u_1^\ell = ie^{-iI_\ell(E, \varepsilon)/h} \sigma_-^\ell v_{-1}^\ell, \end{cases}$$

for some symbols σ_\pm^ℓ such that $\sigma_\pm^\ell = 1 + \mathcal{O}(h)$. After replacing $v_{\pm 1}^\ell$ by $\sigma_\pm^\ell v_{\pm 1}^\ell$ (which does not change the leading asymptotics) we may assume that $\sigma_\pm^\ell = 1$:

$$(4.22) \quad \begin{cases} u_{-1}^\ell = -ie^{iI_\ell(E, \varepsilon)/h} v_1^\ell, \\ u_1^\ell = ie^{-iI_\ell(E, \varepsilon)/h} v_{-1}^\ell, \end{cases}$$

The same discussion applies to the solutions associated to the well to the right. The main rule is simply that the right well becomes the left well of the operator $\tilde{P}_\varepsilon = -h^2 \partial_{\tilde{x}}^2 + V_\varepsilon(-\tilde{x})$ under the change of variables $x = -\tilde{x}$, and we let u_k^r, v_k^r be obtained from the corresponding null solutions $\tilde{u}_k^\ell, \tilde{v}_k^\ell$ of $\tilde{P}_\varepsilon - E$. Note that the Stokes sectors Σ_k^r, S_k^r correspond to the sectors $\tilde{\Sigma}_k^\ell, \tilde{S}_k^\ell$ to the left, defined exactly as Σ_k^ℓ, S_k^ℓ . (Cf. Figure 4.)

This means that we have the 6 solutions $u_k^r, v_k^r, k \in \mathbb{Z}$ which satisfy (4.3) with “ ℓ ” replaced by “ r ” and φ_k^r, ψ_k^r are solutions to the eikonal equation (4.4), vanishing at $z = \alpha_r(E, \varepsilon), z = \beta_r(E, \varepsilon)$ respectively, satisfying (4.5)

with “ ℓ ” replaced by “ r ”. The principal parts $a_{k,0}^r, b_{k,0}^k$ are given by (4.8), (4.10), (4.11), (4.15), (4.17), (4.18) with “ ℓ ” replaced by “ r ”. Here $(V_\varepsilon(x) - E)_r^{\frac{1}{4}}$ is the branch which is ≥ 0 to the right of α_r , when $\varepsilon = 0$ and E is real and close to E_0 . Again, we can modify the choice of u_\pm^r by constant factors $1 + \mathcal{O}(h)$, so that the analogue of (4.13) holds:

$$(4.23) \quad u_0^r = u_{-1}^r + u_1^r.$$

Then we can modify $v_{\pm 1}^r$ by constant factors $1 + \mathcal{O}(h)$ so that (4.22) holds with “ ℓ ” replaced by “ r ”:

$$(4.24) \quad \begin{cases} u_{-1}^r = -ie^{iI_r(E,\varepsilon)/h}v_1^r, \\ u_1^r = ie^{-iI_r(E,\varepsilon)/h}v_{-1}^r, \end{cases}$$

where now (cf. (4.19))

$$(4.25) \quad I_r(E, \varepsilon) = \int_{\beta_r}^{\alpha_r} (E - V_\varepsilon(t))_w^{\frac{1}{2}} dt$$

and $(E - V_\varepsilon)_w^{\frac{1}{2}}$ is now defined near the right well $] \beta_r, \alpha_r[$ as the branch of the square root which is positive on $] \beta_r, \alpha_r[$ when $\varepsilon = 0$ and E is real and close to E_0 .

Notice that this fits with the principle of transforming everything from the right to the left by putting $\tilde{V}_\varepsilon(\tilde{x}) = V_\varepsilon(-\tilde{x})$. \tilde{V}_ε has the left turning points $\tilde{\alpha}_\ell = -\alpha_r, \tilde{\beta}_\ell = -\beta_r$ and

$$\int_{\tilde{\alpha}_\ell}^{\tilde{\beta}_\ell} (E - V_\varepsilon(\tilde{x}))^{\frac{1}{2}} d\tilde{x} = - \int_{\alpha_r}^{\beta_r} (E - V_\varepsilon(x))^{\frac{1}{2}} dx = I_r,$$

with the natural branches of the square root.

Now we build two convenient independent formal WKB solutions w_0^ℓ and w_0^r near the barrier. We set

$$(4.26) \quad w_0^\ell = \frac{1}{2i}(v_1^\ell - v_{-1}^\ell).$$

Since

$$v_1^\ell = i(V_\varepsilon - E)_m^{-\frac{1}{4}} e^{i\psi_1^\ell/h} (1 + \mathcal{O}(h)) = i(V_\varepsilon - E)_m^{-\frac{1}{4}} e^{-i\psi_0^\ell/h} (1 + \mathcal{O}(h)),$$

and

$$v_{-1}^\ell = -i(V_\varepsilon - E)_m^{-\frac{1}{4}} e^{i\psi_1^\ell/h} (1 + \mathcal{O}(h)) = -i(V_\varepsilon - E)_m^{-\frac{1}{4}} e^{-i\psi_0^\ell/h} (1 + \mathcal{O}(h)),$$

we have

$$w_0^\ell = (V_\varepsilon - E)_m^{-\frac{1}{4}} e^{-i\psi_0^\ell/h} (1 + \mathcal{O}(h)).$$

On the other hand, we have

$$v_0^r = (V_\varepsilon - E)_m^{-\frac{1}{4}} e^{i\psi_0^r/h} (1 + \mathcal{O}(h)),$$

so that

$$w_0^\ell = \delta_{\ell,r} e^{J(E,\varepsilon)/h} v_0^r,$$

where $\delta_{\ell,r} = 1 + \mathcal{O}(h)$ is a symbol, and

$$(4.27) \quad J(E, \varepsilon) = -i\psi_0^r - i\psi_0^\ell = \int_{\beta_\ell}^{\beta_r} (V_\varepsilon(t) - E)^{\frac{1}{2}} dt.$$

We now replace v_0^r by $\delta_{\ell,r} v_0^r$ (which does not modify the leading asymptotics) so that

$$(4.28) \quad w_0^\ell = e^{J(E,\varepsilon)/h} v_0^r,$$

Notice that (4.28) fixes a choice for the formal WKB solution v_0^r .

In the same way, we set

$$(4.29) \quad w_0^r = \frac{1}{2i} (v_1^r - v_{-1}^r).$$

and we have

$$w_0^r = \delta_{r,\ell} e^{J(E,\varepsilon)/h} v_0^\ell,$$

then replace v_0^ℓ by $\delta_{r,\ell} v_0^\ell$ and get

$$(4.30) \quad w_0^r = e^{J(E,\varepsilon)/h} v_0^\ell,$$

which we take as the definition of v_0^ℓ .

In analogy with the equation prior to (4.11) we have

$$(4.31) \quad v_0^\ell = \gamma_+^\ell(h) v_1^\ell + \gamma_-^\ell(h) v_{-1}^\ell,$$

$$(4.32) \quad v_0^r = \gamma_+^r(h) v_{-1}^r + \gamma_-^r(h) v_1^r,$$

where $\gamma_\pm^\bullet = 1 + \mathcal{O}(h)$. Having already adjusted v_\pm^\bullet by factors $1 + \mathcal{O}(h)$, there is no place for further adjustments, so we have to refrain from the possibility of replacing γ_\pm^\bullet by 1.

5 WKB expansions of L^2 solutions outside the well

In this section we focus on solutions of the Schrödinger equation (4.1) that are L^2 in a neighborhood of $+\infty$ or $-\infty$ respectively. The existence of such solutions follows from the general theory of partial differential equations since $P_{h,\varepsilon} - E$ is elliptic at infinity for $E \in D(E_0, \varepsilon_0)$. We are interested in their asymptotic behavior as $h \rightarrow 0$.

Let $\delta_0 > 0$. We consider the eikonal (2.6) and transport equations (2.7) on the half-line $]\alpha_r + \delta_0, +\infty[$. There exists $\varepsilon_0 = \varepsilon_0(\delta_0)$ small enough, such that for all $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$, and for $x \in]\alpha_r + \delta_0, +\infty[$, the function

$$(5.1) \quad \varphi_+(x, E) = i \int_{\alpha_r(E, \varepsilon)}^x (V_\varepsilon(t) - E)^{\frac{1}{2}} dt,$$

is a smooth function of x , and an analytic function of (E, ε) , which solves the eikonal equation. We recall that $t \mapsto (V_\varepsilon(t) - E)^{\frac{1}{2}}$ is real and positive in $]\alpha_r + \delta_0, +\infty[$ when $\varepsilon = 0$, so that

$$(5.2) \quad \operatorname{Re}(i\varphi_+(x, E)) < 0.$$

It is then straightforward to obtain the existence of the solutions of the corresponding transport equations, and we get the

Proposition 5.1 *For all $\delta_0 > 0$, there exists $\varepsilon_0 > 0$ such that, for all $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$, the equation (4.1) has a formal WKB solution \tilde{u}_+ in $]\alpha_r + \delta_0, +\infty[$,*

$$(5.3) \quad \tilde{u}_+(x, \varepsilon, E, h) = e^{i\varphi_+(x, E)/h} \sum_{j \geq 0} a_j(x, E, \varepsilon) h^j,$$

where a_j is C^∞ with respect to $x \in]\alpha_2 + \delta_0, +\infty[$, and is holomorphic with respect to $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$. Moreover we can choose a_0 so that,

$$(5.4) \quad a_0(x, E, \varepsilon) = (-i\partial_x \varphi_+)^{-\frac{1}{2}},$$

and we have the estimates, for all $j \geq 0$ and all $k \geq 0$,

$$(5.5) \quad |a_j^{(k)}(x, E, \varepsilon)| = \mathcal{O}(\langle x \rangle^{-\frac{m_0}{4} - j(\frac{m_0}{2} + 1 \operatorname{si}.5) - k}).$$

Proof: We prove (5.5). Differentiating the eikonal equation

$$\varphi'_+(x)^2 = E - V_\varepsilon(x),$$

and using (A2), we easily obtain by induction that, for $k \geq 1$,

$$(5.6) \quad (\varphi'_+)^{(k)}(x) = \mathcal{O}(\langle x \rangle^{\frac{m_0}{2}-k}).$$

Of course we also have, by (A4),

$$\langle x \rangle^{\frac{m_0}{2}} \lesssim |\varphi'_+(x)|,$$

so that (5.4) gives

$$(5.7) \quad \langle x \rangle^{-\frac{m_0}{4}} \lesssim |a_0(x, E, \varepsilon)| \lesssim \langle x \rangle^{-\frac{m_0}{4}}.$$

Then, differentiating the first transport equation

$$(5.8) \quad \varphi'_+(x)a'_0(x, E, \varepsilon) + \frac{\varphi''_+(x)}{2}a_0(x, E, \varepsilon) = 0,$$

we obtain by induction that, uniformly for $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$,

$$(5.9) \quad |a_0^{(k)}(x, E, \varepsilon)| \lesssim \langle x \rangle^{-m_0/4-k},$$

which proves the estimates for $j = 0$ and all $k \in \mathbb{N}$. Now suppose that (5.5) holds for some j and all $k \in \mathbb{N}$. The $(j+1)$ -st transport equation is,

$$(\varphi'_+(x)\partial_x + \frac{i}{2}\varphi''_+(x))a_{j+1} = \frac{i}{2}a''_j,$$

and, setting

$$(5.10) \quad a_{j+1} = f_{j+1}a_0,$$

we get, using also (5.8),

$$(5.11) \quad (a_0(x)\varphi'_+(x))f'_{j+1}(x) = \frac{i}{2}a''_j(x).$$

Thus we have first

$$(5.12) \quad f_{j+1}(x) = \frac{i}{2} \int_{+\infty}^x \frac{a''_j(t)}{\varphi'_+(t)a_0(t)} dt = \mathcal{O}(\langle x \rangle^{-(j+1)(\frac{m_0}{2}+1)}),$$

and, differentiating (5.11), we obtain by induction

$$(5.13) \quad f_{j+1}^{(k)}(x) = \mathcal{O}(\langle x \rangle^{-(j+1)(\frac{m_0}{2}+1)-k}).$$

Then (5.5) follows by differentiating (5.10) and using Leibniz formula. \square

To the formal series $\sum_{j \geq 0} a_j h^j$ defined in Proposition 5.1, we can associate a function a by means of a Borel construction, setting

$$(5.14) \quad a(x, E, \varepsilon, h) = \sum_{j \geq 0} a_j(x, E, \varepsilon) h^j \chi(\lambda_j h)$$

for some plateau function $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ over $\{0\}$, and a suitable sequence (λ_j) of real numbers such that $\lambda_j \rightarrow +\infty$ as $j \rightarrow +\infty$ (see e.g. [12, Chapter 2]). Then, for all $N \in \mathbb{N}$ and any $k \geq 0$,

$$(5.15) \quad |a^{(k)}(x, h) - \sum_{j=0}^{N-1} a_j^{(k)}(x) h^j| = \mathcal{O}(h^N \langle x \rangle^{-\frac{m_0}{4} - N(\frac{m_0}{2}+1)-k}).$$

Moreover $u_{+,wkb} = e^{i\varphi_+/h} a$ is an approximate solution to the Schrödinger equation (4.1), in the sense that

$$(5.16) \quad P_{h,\varepsilon} u_{+,wkb}(x, E, \varepsilon, h) = e^{i\varphi_+(x,E,\varepsilon)/h} r(x, E, \varepsilon, h),$$

where, for all $N \in \mathbb{N}$,

$$(5.17) \quad r(x, E, \varepsilon, h) = \mathcal{O}(h^N \langle x \rangle^{-N}).$$

Now we build a solution u_+ that has the formal WKB solution constructed above as an asymptotic expansion in $]\alpha_r + \delta_0, +\infty[$. To do so, we establish first some estimates for the solutions of the inhomogeneous Schrödinger equation

$$(5.18) \quad -h^2 u'' + (V_\varepsilon - E)u = v,$$

on intervals of the form $I_\lambda = [\frac{\lambda}{2}, \frac{3\lambda}{2}]$, for large λ . For simpler notations we write

$$(5.19) \quad Q(x) = Q_{E,\varepsilon}(x) = V_\varepsilon - E,$$

and we set

$$(5.20) \quad x = \lambda + \lambda \tilde{x},$$

so that $\tilde{x} \in [-\frac{1}{2}, \frac{1}{2}]$. Multiplying also by λ^{-m_0} , the equation (5.18) on I_λ is equivalent to the equation

$$(5.21) \quad (\tilde{h}^2 D_{\tilde{x}}^2 + \tilde{Q}(\tilde{x}))\tilde{u} = \tilde{v},$$

on $[-\frac{1}{2}, \frac{1}{2}]$, where

$$(5.22) \quad \tilde{h} = \frac{h}{\lambda^{1+m_0/2}}, \quad \tilde{Q}(\tilde{x}) = \lambda^{-m_0}Q(x), \quad \tilde{v}(\tilde{x}) = \lambda^{-m_0}v(x).$$

Notice in particular that $\tilde{Q} \asymp 1$, and that $\tilde{Q}^{(k)} = \mathcal{O}(1)$ for all $k \geq 1$. As in [23, Chapter 7], we write (5.21) as the first order system,

$$(5.23) \quad (\tilde{h}D_{\tilde{x}} + A(\tilde{x}))U = V, \quad A(\tilde{x}) = \begin{pmatrix} 0 & -1 \\ \tilde{Q}(\tilde{x}) & 0 \end{pmatrix}, \quad U = \begin{pmatrix} \tilde{u} \\ \tilde{h}D_{\tilde{x}}\tilde{u} \end{pmatrix}, \quad V = \begin{pmatrix} 0 \\ \tilde{v} \end{pmatrix},$$

and we denote $\tilde{\mathcal{E}} = (\tilde{\mathcal{E}}_{i,j}) \in \mathcal{C}^\infty(I \times I, \mathcal{M}_2(\mathbb{C}))$ the fundamental solution of this system. One can prove that (see [23, Theorem 7.1.3]), for any $j, k \in N$,

$$(5.24) \quad \|(h\partial_{\tilde{x}})^j (h\partial_{\tilde{x}})^k \tilde{\mathcal{E}}(\tilde{x}, \tilde{y})\| \leq C_{j,k} \exp\left(\frac{1}{\tilde{h}} |\operatorname{Im} \tilde{\varphi}(\tilde{x}) - \operatorname{Im} \tilde{\varphi}(\tilde{y})|\right),$$

for some $C_{j,k} > 0$, where $\tilde{\varphi}$ is the solution of the eikonal equation associated to (5.21) such that $e^{i\tilde{\varphi}(\tilde{x})/\tilde{h}}$ is decaying as \tilde{x} increases. Now the solution \tilde{u} of (5.21) satisfies, for any $\tilde{x}, \tilde{y} \in [-\frac{1}{2}, \frac{1}{2}]$,

$$(5.25) \quad \begin{pmatrix} \tilde{u}(\tilde{x}) \\ \tilde{h}D_{\tilde{x}}\tilde{u}(\tilde{x}) \end{pmatrix} = \tilde{\mathcal{E}}(\tilde{x}, \tilde{y}) \begin{pmatrix} \tilde{u}(\tilde{y}) \\ \tilde{h}D_{\tilde{x}}\tilde{u}(\tilde{y}) \end{pmatrix}.$$

Since $i\tilde{\varphi}(\tilde{x})/\tilde{h} = i\varphi(x)/h$, where φ is the solution of the eikonal equation associated to (5.18) which decays when x increases, we also have, with $u(x) = \tilde{u}(\tilde{x})$,

$$(5.26) \quad \begin{pmatrix} u(x) \\ \frac{h}{\lambda^{m_0}} D_x u(x) \end{pmatrix} = \tilde{\mathcal{E}}(\tilde{x}, \tilde{y}) \begin{pmatrix} u(y) \\ \frac{h}{\lambda^{m_0}} D_y u(y) \end{pmatrix},$$

with

$$(5.27) \quad \|\tilde{\mathcal{E}}(\tilde{x}, \tilde{y})\| \leq C \exp\left(\frac{1}{h} |\operatorname{Im} \varphi(x) - \operatorname{Im} \varphi(y)|\right).$$

Replacing λ by $|x|$ we get

$$(5.28) \quad \begin{pmatrix} u(x) \\ hDu(x) \end{pmatrix} = \mathcal{E}(x, y) \begin{pmatrix} u(y) \\ hDu(y) \end{pmatrix},$$

where

$$(5.29) \quad \mathcal{E}(x, y) = \begin{pmatrix} 1 & 0 \\ 0 & |x|^{m_0/2} \end{pmatrix} \hat{\mathcal{E}}(x, y) \begin{pmatrix} 1 & 0 \\ 0 & |y|^{-m_0/2} \end{pmatrix},$$

and $\hat{\mathcal{E}}$ satisfies the estimate (5.27) possibly with another constant $C > 0$.

For general $\alpha_r + \delta_0 \leq x \leq y$, we can cover $[x, y]$ with $1 + \mathcal{O}(\ln(\frac{y}{x}))$ intervals of the type I_λ . Thus, writing

$$\mathcal{E}(x, y) = \mathcal{E}(x, x_1) \mathcal{E}(x_1, x_2) \dots \mathcal{E}(x_n, y),$$

where each of the intervals $[x_j, x_{j+1}]$ is contained in one of the chosen I_λ 's, we obtain

$$(5.30) \quad \|\mathcal{E}(x, y)\| \leq C^{1+\mathcal{O}(\ln(\frac{y}{x}))} \exp\left(\frac{1}{h} |\operatorname{Im} \varphi(x) - \operatorname{Im} \varphi(y)| y^{-m_0/2}\right).$$

In particular we have, for all $\alpha_r + \delta_0 \leq x \leq y$,

$$(5.31) \quad |\mathcal{E}_{12}(x, y)| = \frac{\mathcal{O}(1)}{h} \frac{y^{C-m_0/2}}{x^C} \exp\left(\frac{1}{h} \operatorname{Im}(\varphi(y) - \varphi(x))\right),$$

where we have used the fact that for $x \leq y$, $\operatorname{Im} \varphi(y) \geq \operatorname{Im} \varphi(x)$.

Now we consider again the function $u_{+,wkb}$, and we denote u_λ the unique solution of the Schrödinger equation (4.1) such that

$$(5.32) \quad \begin{cases} u_\lambda(\lambda, E, \varepsilon, h) = u_{+,wkb}(\lambda, E, \varepsilon, h), \\ hDu_\lambda(\lambda, E, \varepsilon, h) = hDu_{+,wkb}(\lambda, E, \varepsilon, h). \end{cases}$$

We have

$$(5.33) \quad P_{h,\varepsilon}(1_{[\alpha_r+\delta_0,\lambda]}(u_\lambda - u_{+,wkb})) = 1_{[\alpha_r+\delta_0,\lambda]} r,$$

so that, for $x \in [\alpha_r + \delta_0, \lambda]$,

$$(5.34) \quad u_\lambda(x) - u_{+,wkb}(x) = -\frac{i}{h} \int_x^\lambda \mathcal{E}_{(1,2)}(x, y) r(y) dy.$$

Then, noticing that we can take $C > 0$ arbitrarily large in (5.31), we get, for all $N \in \mathbb{N}$ and all $k \in \mathbb{N}$,

$$(5.35) \quad u_{\lambda}^{(k)}(x) - u_{+,wkb}^{(k)}(x) = \mathcal{O}(h^N \langle x \rangle^{-N} e^{-\operatorname{Im} \varphi(x)/h}),$$

and, for $\lambda_1 < \lambda_2 \in \mathbb{R}^+$ large enough,

$$(5.36) \quad u_{\lambda_2}^{(k)}(x) - u_{\lambda_1}^{(k)}(x) = \mathcal{O}(h^N \langle x \rangle^{-N} \lambda_1^{-N} e^{-\operatorname{Im} \varphi(x)/h}),$$

Thus, the family (u_{λ}) converges to some function u_+ , which is an exact solution to (4.1), and (5.35) gives that, for all $N \in \mathbb{N}$ and all $k \in \mathbb{N}$,

$$(5.37) \quad u_+^{(k)}(x) - u_{+,wkb}^{(k)}(x) = \mathcal{O}(h^N \langle x \rangle^{-N} e^{-\operatorname{Im} \varphi(x)/h}).$$

We have proved the main part of the

Proposition 5.2 *Let $\delta_0 > 0$, and $\varepsilon_0 > 0$ be small enough. Let $\tilde{u} = e^{i\varphi_+/h} \sum_{j \geq 0} a_j h^j$ be a formal WKB solution in $] \alpha_r + \delta_0, +\infty[$ satisfying (5.1) and (5.4). Then, for any $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$, the equation (4.1) has a unique solution u_+ on $] \alpha_r + \delta_0, +\infty[$ such that,*

$$(5.38) \quad u_+(x, E, \varepsilon, h) = a_+(x, E, \varepsilon, h) e^{i\varphi_+(x, E, \varepsilon)/h}$$

with

$$(5.39) \quad a_+(x, E, \varepsilon, h) \sim \sum_{j=0}^{\infty} a_j^+(x, E, \varepsilon) h^j,$$

in the sense that

$\forall N \in \mathbb{N}^*, \forall k \in \mathbb{N}, \exists C_{N,k} > 0$ such that

$$(5.40) \quad |\partial_x^k \left(a_+(x, h) - \sum_{j=0}^{N-1} a_j^+(x) h^j \right)| \leq C_{N,k} h^N \langle x \rangle^{-\frac{m_0}{4} - N(\frac{m_0}{2} + 1) - k}.$$

Moreover u_+ belongs to $L^2(] \alpha_r + \delta_0, +\infty[)$, and it is analytic with respect to $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$.

Proof: It only remains to prove that the solution u_+ belongs to $L^2(] \alpha_r + \delta_0, +\infty[)$. Assumption (A2) implies that there exists $C > 0$ such that

$\operatorname{Re}(V_\varepsilon(x) - E) > \frac{1}{C^2}$ for all x large enough. Thus we have, for $x \in]\alpha_2, +\infty[$ large enough,

$$(5.41) \quad \operatorname{Re}(i\varphi_+(x)) = -\operatorname{Re} \int_{\alpha_r}^x (V_\varepsilon(t) - E)^{\frac{1}{2}} dt \leq -\frac{x}{C} + C.$$

On the other hand, the estimate (5.40) for $N = 0$, $k = 0$, gives $a_+(x, E, \varepsilon) = \mathcal{O}(\langle x \rangle^{-m_0/4})$, so that $u_+ \in L^2(]\alpha_r + \delta_0, +\infty[)$. \square

It is clear that we have the same result for the existence of a solution $u_- \in L^2(\mathbb{R}^-)$ that has, for any $\delta_0 > 0$, a WKB asymptotic expansion in $]-\infty, \alpha_\ell - \delta_0[$ of the form

$$(5.42) \quad u_-(x, E, \varepsilon, h) = a_-(x, E, \varepsilon, h) e^{i\varphi_-(x, E, \varepsilon)/h},$$

where the phase φ_- is defined by

$$(5.43) \quad i\varphi_-(x, E, \varepsilon) = \int_{\alpha_\ell(E, \varepsilon)}^x (V_\varepsilon(t) - E)^{\frac{1}{2}} dt$$

where we recall that the determination of $t \mapsto (V_\varepsilon(t) - E)^{\frac{1}{2}}$ is fixed in such a way that, for $x \in]-\infty, \alpha_\ell - \delta_0[$,

$$(5.44) \quad \operatorname{Re}(i\varphi_-(x, E, \varepsilon)) < 0.$$

We also have, in the same sense as in (5.40),

$$(5.45) \quad a_-(x, E, \varepsilon, h) \sim \sum_{j=0}^{\infty} a_j^-(x, E, \varepsilon) h^j,$$

where $u_{wkb} = e^{i\varphi_-/h} \sum_{j=0}^{\infty} a_j^- h^j$ is a formal WKB solution. It is of course also analytic with respect to $(E, \varepsilon) \in D(E_0, \varepsilon_0) \times D(0, \varepsilon_0)$.

6 The quantization condition

To start with, we derive the quantization condition, using only the double well structure but not yet the \mathcal{PT} -symmetry nor the symmetry following from the fact that P_0 is real and self-adjoint.

In Section 5 we have introduced the two null solutions u_+ , u_- of $(P_\varepsilon - E)u = 0$ that decay exponentially near $+\infty$ and $-\infty$ respectively, and we know that E is an eigenvalue of P_ε precisely when $W(u_+, u_-) = 0$ or equivalently when u_+ and u_- are colinear. It is clear that we can choose u_\pm and u_0^ℓ , u_0^r of the preceding section, so that

$$u_0^\ell = u_-, \quad u_0^r = u_+.$$

By (4.13), (4.22) we have

$$(6.1) \quad u_0^\ell = -ie^{iI_\ell/h}v_1^\ell + ie^{-iI_\ell/h}v_{-1}^\ell.$$

Similarly, by (4.23), (4.24),

$$(6.2) \quad u_0^r = -ie^{iI_r/h}v_1^r + ie^{-iI_r/h}v_{-1}^r.$$

Here, we recall (4.26), (4.28), implying

$$(6.3) \quad v_0^r = e^{-J/h} \frac{1}{2i} (v_1^\ell - v_{-1}^\ell)$$

and (4.29), (4.30), that give

$$(6.4) \quad v_0^\ell = e^{-J/h} \frac{1}{2i} (v_1^r - v_{-1}^r).$$

(4.31) and (6.3) form a system that allows to express $v_{\pm 1}^\ell$ in terms of v_0^r , v_0^ℓ . Similarly, (4.32) and (6.4) allow us to express v_\pm^r in terms of v_0^r , v_0^ℓ . After some straightforward calculations, we get,

$$(6.5) \quad \begin{pmatrix} v_1^\ell \\ v_{-1}^\ell \end{pmatrix} = \frac{1}{\gamma_-^\ell + \gamma_+^\ell} \begin{pmatrix} 1 & 2ie^{J/h}\gamma_-^\ell \\ 1 & -2ie^{J/h}\gamma_+^\ell \end{pmatrix} \begin{pmatrix} v_0^\ell \\ v_0^r \end{pmatrix},$$

$$(6.6) \quad \begin{pmatrix} v_1^r \\ v_{-1}^r \end{pmatrix} = \frac{1}{\gamma_-^r + \gamma_+^r} \begin{pmatrix} 2ie^{J/h}\gamma_+^r & 1 \\ -2ie^{J/h}\gamma_-^r & 1 \end{pmatrix} \begin{pmatrix} v_0^\ell \\ v_0^r \end{pmatrix}.$$

Combining (6.1) and (6.5), we get after a straightforward calculation,

$$(6.7) \quad u_0^\ell = \frac{1}{\gamma_-^\ell + \gamma_+^\ell} \left(\frac{1}{i} (e^{iI_\ell/h} - e^{-iI_\ell/h}) \quad 2e^{J/h} (e^{iI_\ell/h}\gamma_-^\ell + e^{-iI_\ell/h}\gamma_+^\ell) \right) \begin{pmatrix} v_0^\ell \\ v_0^r \end{pmatrix}.$$

Combining (6.2), (6.6), we get
(6.8)

$$u_0^r = \frac{1}{\gamma_-^r + \gamma_+^r} \left(2e^{J/h} \left(e^{iI_r/h} \gamma_+^r + e^{-iI_r/h} \gamma_-^r \right) - \frac{1}{i} \left(e^{iI_r/h} - e^{-iI_r/h} \right) \right) \begin{pmatrix} v_0^\ell \\ v_0^r \end{pmatrix}.$$

Since v_0^ℓ, v_0^r are linearly independent, we see that E is an eigenvalue of P_ε precisely when the two row matrices in (6.7) and (6.8) are colinear or equivalently when the determinant of the matrix, formed by these two rows, is equal to 0. We then get the quantization condition

$$0 = \frac{1}{i} \left(e^{iI_\ell/h} - e^{-iI_\ell/h} \right) \frac{1}{i} \left(e^{iI_r/h} - e^{-iI_r/h} \right) - 4e^{2J/h} \left(e^{iI_\ell/h} \gamma_-^\ell + e^{-iI_\ell/h} \gamma_+^\ell \right) \left(e^{iI_r/h} \gamma_+^r + e^{-iI_r/h} \gamma_-^r \right),$$

which we rewrite as

$$(6.9) \quad f(E, \varepsilon) = 0,$$

where

$$(6.10) \quad f(E, \varepsilon) = \frac{1}{4} \left(e^{iI_\ell/h} \gamma_-^\ell + e^{-iI_\ell/h} \gamma_+^\ell \right) \left(e^{iI_r/h} \gamma_+^r + e^{-iI_r/h} \gamma_-^r \right) - \frac{1}{4} e^{-2J/h} \sin(I_\ell/h) \sin(I_r/h).$$

We shall now take into account the various symmetry properties. For functions $u(x, E, \varepsilon)$, where x, E vary in some domains in \mathbb{C} and ε in some real domain, we put,

$$(6.11) \quad \text{Co}(u)(x, E, \varepsilon) = u^*(x, E, \varepsilon) = \overline{u(\bar{x}, \bar{E}, -\varepsilon)},$$

$$(6.12) \quad \text{Pt}(u)(x, E, \varepsilon) = u^\dagger(x, E, \varepsilon) = \overline{u(-\bar{x}, \bar{E}, \varepsilon)},$$

so that Pt is equal to \mathcal{PT} in the introduction. Notice that Pt and Co are idempotent anti-linear operators that commute: $\text{Co} \circ \text{Pt} = \text{Pt} \circ \text{Co}$.

Using only that $V_\varepsilon = V_0 + i\varepsilon W$ with V_0, W real-valued on the real domain, we see that

$$V_\varepsilon^*(x) = \overline{V_{-\varepsilon}(\bar{x})} = V_\varepsilon(x), \quad \text{Pt}(V_\varepsilon)(x) = \overline{V_\varepsilon(-\bar{x})} = V_0(-x) - i\varepsilon W(-x),$$

and if we make the \mathcal{PT} -symmetry assumption (A5), we get $\text{Pt}(V_\varepsilon) = V_\varepsilon$ and hence that

$$(6.13) \quad (P_\varepsilon - E) \circ \text{Pt} = \text{Pt} \circ (P_\varepsilon - E).$$

Without (A5), we still have

$$(6.14) \quad (P_\varepsilon - E) \circ \text{Co} = \text{Co} \circ (P_\varepsilon - E).$$

To verify this quickly, we observe that $\text{Co}(uv) = \text{Co}(u)\text{Co}(v)$ for products of functions and similarly for Pt , and that $\text{Pt} \circ \partial_x = -\partial_x \circ \text{Pt}$, $\text{Co} \circ \partial_x = \partial_x \circ \text{Co}$. Recall that to leading order,

$$u_0^\ell \equiv u_{0,0}^\ell := (V_\varepsilon - E)_\ell^{-\frac{1}{4}} e^{\frac{1}{\hbar} \int_{\alpha_\ell}^x (V_\varepsilon - E)_\ell^{\frac{1}{2}} dt}.$$

By straightforward calculations, observing that $\alpha_\ell(\overline{E}, -\varepsilon) = \overline{\alpha_\ell(E, \varepsilon)}$ (i.e. $\alpha_\ell^* = \alpha_\ell$), we obtain,

$$(6.15) \quad \text{Co}(u_{0,0}^\ell) = u_{0,0}^\ell.$$

In view of (6.14), we know that $\text{Co}(u_0^\ell)$ is a null solution of $P_\varepsilon - E$ and using also (6.15), we conclude that $\frac{1}{2}(u_0^\ell + \text{Co}(u_0^\ell))$ is a null solution with leading asymptotics $u_{0,0}^\ell$ which is invariant under Co , so if we replace u_0^ℓ by this function we gain the property,

$$(6.16) \quad \text{Co}(u_0^\ell) = u_0^\ell.$$

Similarly, in the discussion leading to (4.12) we see that we can choose $u_{\pm 1}^\ell$ so that

$$(6.17) \quad u_1^\ell = \text{Co}(u_{-1}^\ell).$$

Since u_{-1}^ℓ, u_1^ℓ form a basis for the space of null solutions of $P_\varepsilon - E$, we get from (4.12), (6.15), that $\text{Co}(\tau_+) = \tau_-$, so after replacing $u_{\mp 1}^\ell$ by $\tau_\pm u_{\mp 1}^\ell$, we still have (6.17) for the new functions $u_{\mp 1}^\ell$ in (4.13).

Next, notice that I_ℓ in (4.19) satisfies

$$(6.18) \quad I_\ell^* = I_\ell.$$

This means that

$$(6.19) \quad v_1^\ell = \text{Co}(v_{-1}^\ell),$$

for $v_{\pm 1}^\ell$ in (4.22).

The whole discussion so far applies with “ ℓ ” replaced by “ r ” and we get

$$(6.20) \quad \text{Co}(u_0^r) = u_0^r, \quad I_r^* = I_r, \quad u_1^r = \text{Co}(u_{-1}^r), \quad v_1^r = \text{Co}(v_{-1}^r).$$

Moreover, we check that

$$(6.21) \quad J^* = J.$$

From (4.26), (4.28) we now get

$$(6.22) \quad \text{Co}(v_0^r) = v_0^r.$$

Similarly,

$$(6.23) \quad \text{Co}(v_0^\ell) = v_0^\ell.$$

Then in (4.31), (4.32) we must have

$$(6.24) \quad \text{Co}(\gamma_+^\ell) = \gamma_-^\ell, \quad \text{Co}(\gamma_+^r) = \gamma_-^r.$$

It follows that f in (6.9), (6.10) satisfies

$$(6.25) \quad f^* = f.$$

Let us finally use the \mathcal{PT} -symmetry assumption (A5) or equivalently (6.13). We then check that

$$(6.26) \quad I_\ell^\dagger = I_r,$$

and

$$(6.27) \quad J^\dagger = J,$$

and that we can choose

$$(6.28) \quad u_0^r = \text{Pt}(u_0^\ell), \quad u_1^r = \text{Pt}(u_{-1}^\ell), \quad u_{-1}^r = \text{Pt}(u_1^\ell),$$

$$(6.29) \quad v_{\pm 1}^r = \text{Pt}(v_{\mp 1}^\ell).$$

Then by (6.3), (6.4),

$$(6.30) \quad v_0^r = \text{Pt}(v_0^\ell),$$

and from (4.31), (4.32) we infer that

$$(6.31) \quad \gamma_\pm^r = \text{Pt}(\gamma_\pm^\ell).$$

It follows that

$$(6.32) \quad f^\dagger = f.$$

We have seen that the zeros of $f(\cdot, \varepsilon)$ coincide with the eigenvalues of P_ε in a neighborhood of E_0 . We end this section by showing that the multiplicities agree also.

Recall (6.7), (6.8) that we write as

$$\begin{aligned} u_0^\ell &= a^\ell v_0^\ell + b^\ell v_0^r, \\ u_0^r &= a^r v_0^\ell + b^r v_0^r. \end{aligned}$$

Taking the Wronskians, we get

$$W(u_0^\ell, u_0^r) = \det \begin{pmatrix} a^\ell & b^\ell \\ a^r & b^r \end{pmatrix} W(v_0^\ell, v_0^r).$$

Here the last Wronskian is non-vanishing, so up to a non-vanishing holomorphic factor f is equal to $W(u_0^\ell, u_0^r)$ and the zeros of f , counted with their multiplicity coincide with those of $W(v_0^\ell, v_0^r)$.

Hence it remains to identify eigenvalues of P_ε counted with their multiplicity with the zeros of the Wronskian $W(u_0^\ell, u_0^r)$. For that we can widen the perspective slightly and apply a general discussion:

Let $a \in \mathbb{R}$. Let λ vary in $\text{neigh}(E_0, \mathbb{C})$. (The symbol “ E ” will temporarily be used to denote operators.) Using the ellipticity of $P_\varepsilon - \lambda$ near $+\infty$, we see that the right Dirichlet problem

$$(P_\varepsilon - \lambda)u = v, \quad u(a) = v_+$$

has a unique solution $u \in H^2(]a, +\infty[)$ for every $(v, v_+) \in H^0(]a, +\infty[) \times \mathbb{C}$. Similarly, by using the ellipticity near $-\infty$ we see that the corresponding

left Dirichlet problem has a unique solution $u \in H^2([-\infty, a])$ for every $(v, v_+) \in H^0([-\infty, a]) \times \mathbb{C}$. Denote the solutions to the two problems by $u = E_r v + E_r^+ v_+$ and $u = E_\ell v + E_\ell^+ v_+$ respectively.

It follows that the Grushin problem

$$\begin{cases} (P_\varepsilon - \lambda)u + R_- u_- = v, \\ R_+ u = v_+, \end{cases}$$

has a unique solution

$$(u, u_-) \in ((H^2([-\infty, a]) \oplus H^2([a, +\infty])) \cap H^1(\mathbb{R})) \times \mathbb{C}$$

for every $(v, v_+) \in H^0(\mathbb{R}) \times \mathbb{C}$, where

$$R_+ u := u(a), \quad R_- u_- = u_- \delta_a,$$

and δ_a denotes the delta function at $x = a$. Indeed, the solution is given by

$$u(x) = \begin{cases} E_\ell v + E_\ell^+ v_+, & x < a \\ E_r v + E_r^+ v_+, & x > a, \end{cases} \quad u_- = (h^2 \partial_z u)(a-0) - (h^2 \partial_z u)(a+0).$$

We write this solution,

$$\begin{pmatrix} u \\ u_- \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} \begin{pmatrix} v \\ v_+ \end{pmatrix}.$$

It is a standard fact for the Grushin reduction (see [16, Section 6, Appendix A], or [24]) that the eigenvalues counted with their multiplicity, coincide (near E_0) with the zeros of $E_{-+}(z)$ counted with their multiplicity (ε is here fixed and suppressed from the notation most of the time). For completeness, we recall the proof. Let z_0 be an eigenvalue of P . Its multiplicity $m(z_0)$ is equal to the rank, and hence to the trace of the spectral projection

$$m(z_0) = \text{tr} \frac{1}{2i\pi} \int_\gamma (z - P)^{-1} dz,$$

where γ is the oriented boundary of a small disc centered at z_0 . Now

$$(z - P)^{-1} = -E(z) + E_+(z)E_{-+}^{-1}(z)E_-(z),$$

and $E(z)$ is holomorphic near z_0 , so

$$\begin{aligned}
(6.33) \quad m(z_0) &= \operatorname{tr} \frac{1}{2i\pi} \int_{\gamma} E_+(z) E_{-+}^{-1}(z) E_-(z) dz \\
&= \frac{1}{2i\pi} \int_{\gamma} \operatorname{tr}(E_+(z) E_{-+}^{-1}(z) E_-(z)) dz \\
&= \frac{1}{2i\pi} \int_{\gamma} \operatorname{tr}(E_{-+}^{-1}(z) E_-(z) E_+(z)) dz \\
&= \frac{1}{2i\pi} \int_{\gamma} E_{-+}^{-1}(z) E_-(z) E_+(z) dz.
\end{aligned}$$

Finally, since $E_-(z) E_+(z) = \partial_z E_{-+}^{-1}(z)$, we see that $m(z_0)$ is equal to the multiplicity of z_0 as a zero of E_{-+} .

Denoting $u_- = E_{\ell}^+(1)$, $u_+ = E_r^+(1)$, we notice that

$$E_{-+} = h^2(\partial_z u_-(a) - \partial_z u_+(a)) = hW(u_-, u_+),$$

since $u_{\mp}(a) = 1$. Thus, in a neighborhood of E_0 , the eigenvalues of P_{ε} counted with their multiplicity can be identified with the zeros of $\lambda \mapsto W(u_-(\lambda), u_+(\lambda))$.

If $\operatorname{neigh}(E_0, \mathbb{C}) \ni \lambda \mapsto \tilde{u}_{\mp}(z, \lambda)$ are holomorphic families of null solutions to $P_{\varepsilon} - \lambda$, exponentially decaying near $\mp\infty$ and $\neq 0$, $\forall \lambda$, then $\tilde{u}_{\mp} = \sigma_{\mp}(\lambda) u_{\mp}$, where σ_{\mp} are holomorphic in λ and non-vanishing. Thus the zeros of $W(\tilde{u}_-, \tilde{u}_+) = \sigma_-(\lambda) \sigma_+(\lambda) W(u_-, u_+)$ coincides with those of $W(u_-, u_+)$ and we have completed the identification.

7 The behaviour of the eigenvalues

In order to study the zeros of $f(\cdot, \varepsilon)$, we first recollect the various symmetries:

$$(7.1) \quad J^* = J = J^{\dagger}, \quad I_{\ell}^* = I_{\ell}, \quad I_r^* = I_r, \quad I_{\ell}^{\dagger} = I_r,$$

and

$$(7.2) \quad \left(\gamma_{-}^{\ell}\right)^* = \gamma_{+}^{\ell}, \quad \left(\gamma_{-}^r\right)^* = \gamma_{+}^r, \quad \left(\gamma_{\pm}^{\ell}\right)^{\dagger} = \gamma_{\pm}^r,$$

where we recall that $\gamma_{\pm}^{\bullet} = 1 + \mathcal{O}(h)$.

Let us first look at the factor

$$(7.3) \quad g = g_{\ell}(E, \varepsilon) = \left(e^{\frac{i}{h} I_{\ell}} \gamma_{-}^{\ell} + e^{-\frac{i}{h} I_{\ell}} \gamma_{+}^{\ell} \right)$$

and drop the super/subscript ℓ when convenient to do so. From (7.1), (7.2), we infer that

$$(7.4) \quad g^{*} = g$$

Write

$$(7.5) \quad \begin{aligned} \gamma_{-}^{\ell} &= \left(\gamma_{-}^{\ell} \gamma_{+}^{\ell} \right)^{\frac{1}{2}} \left(\gamma_{-}^{\ell} / \gamma_{+}^{\ell} \right)^{\frac{1}{2}} =: \rho_{\ell} e^{i\theta_{\ell}} \\ \gamma_{+}^{\ell} &= \left(\gamma_{-}^{\ell} \gamma_{+}^{\ell} \right)^{\frac{1}{2}} \left(\gamma_{-}^{\ell} / \gamma_{+}^{\ell} \right)^{-\frac{1}{2}} =: \rho_{\ell} e^{-i\theta_{\ell}}, \end{aligned}$$

where we choose the branches of the square roots close to 1 and the logarithm close to 0, so that $\rho = 1 + \mathcal{O}(h)$, $\theta = \mathcal{O}(h)$. Then

$$(7.6) \quad \rho^{*} = \rho,$$

so $(e^{i\theta})^{*} = e^{-i\theta}$ and hence

$$(7.7) \quad \theta^{*} = \theta.$$

We write

$$(7.8) \quad g_{\ell} = \rho_{\ell} (e^{\frac{i}{h} \tilde{I}_{\ell}} + e^{-\frac{i}{h} \tilde{I}_{\ell}}), \quad \tilde{I}_{\ell} = I_{\ell} + h\theta_{\ell} = I_{\ell} + \mathcal{O}(h^2) = \tilde{I}_{\ell}^{*}.$$

Similarly, we consider

$$(7.9) \quad g = g_r(E, \varepsilon) = \left(e^{\frac{i}{h} I_r} \gamma_{+}^r + e^{-\frac{i}{h} I_r} \gamma_{-}^r \right).$$

and again we have (7.4), now with $g = g_r$. Write

$$(7.10) \quad \begin{aligned} \gamma_{+}^r &= \left(\gamma_{-}^r \gamma_{+}^r \right)^{\frac{1}{2}} \left(\gamma_{+}^r / \gamma_{-}^r \right)^{\frac{1}{2}} =: \rho_r e^{i\theta_r} \\ \gamma_{-}^r &= \left(\gamma_{-}^r \gamma_{+}^r \right)^{\frac{1}{2}} \left(\gamma_{+}^r / \gamma_{-}^r \right)^{-\frac{1}{2}} =: \rho_r e^{-i\theta_r}. \end{aligned}$$

again with $\rho = 1 + \mathcal{O}(h)$, $\theta = \mathcal{O}(h)$ satisfying (7.6), (7.7).

We write

$$(7.11) \quad g_r = \rho_r(e^{\frac{i}{h}\tilde{I}_r} + e^{-\frac{i}{h}\tilde{I}_r}), \quad \tilde{I}_r = I_r + h\theta_r = I_r + \mathcal{O}(h^2) = \tilde{I}_r^*.$$

We now take into account the \mathcal{PT} symmetry. Clearly,

$$(7.12) \quad \rho_\ell^\dagger = \rho_r$$

and from $(\gamma_-^\ell)^\dagger = \gamma_-^r$, we get $\rho_r e^{-i\theta_\ell^\dagger} = \rho_r e^{-i\theta_r}$, so

$$(7.13) \quad \theta_\ell^\dagger = \theta_r \text{ and hence } \tilde{I}_\ell^\dagger = \tilde{I}_r.$$

Using also that $I_\ell^\dagger = I_r$, we can rewrite f in (6.10) as

$$\begin{aligned} f(E, \varepsilon) &= \frac{\rho \rho^\dagger}{4} \left(e^{\frac{i}{h}\tilde{I}} + e^{-\frac{i}{h}\tilde{I}} \right) \left(e^{\frac{i}{h}\tilde{I}^\dagger} + e^{-\frac{i}{h}\tilde{I}^\dagger} \right) \\ &\quad - \frac{1}{4} e^{-2J/h} \sin(I/h) \sin(I^\dagger/h) \\ &= \rho \rho^\dagger \cos(\tilde{I}/h) \cos(\tilde{I}^\dagger/h) - \frac{1}{4} e^{-2J/h} \sin(I/h) \sin(I^\dagger/h) \end{aligned}$$

where $\tilde{I} = \tilde{I}_\ell$, $I = I_\ell$, $\rho = \rho_\ell$. Dividing this function with $\rho \rho^\dagger$ will not modify the zeros and we get the new (slightly modified) function that we shall denote by the same symbol,

$$(7.14) \quad f(E, \varepsilon) = \cos(\tilde{I}/h) \cos(\tilde{I}^\dagger/h) - \frac{1}{4} e^{-2\tilde{J}/h} \sin(I/h) \sin(I^\dagger/h),$$

where

$$(7.15) \quad \tilde{J} = J + h \ln(\rho \rho^\dagger) = J + \mathcal{O}(h^2).$$

We know that

$$(7.16) \quad f^\dagger = f = f^*.$$

From

$$(7.17) \quad I(E, \varepsilon) = \int_{\alpha_\ell}^{\beta_\ell} (E - V_\varepsilon(x))^{\frac{1}{2}} dx,$$

we get,

$$(7.18) \quad \partial_E I(E, \varepsilon) = \frac{1}{2} \int_{\alpha_\ell}^{\beta_\ell} (E - V_\varepsilon(x))^{-\frac{1}{2}} dx,$$

and

$$(7.19) \quad \partial_\varepsilon I(E, \varepsilon) = \frac{1}{2i} \int_{\alpha_\ell}^{\beta_\ell} (E - V_\varepsilon(x))^{-\frac{1}{2}} W(x) dx.$$

It follows that

$$(7.20) \quad \partial_E I(E, 0) > 0, \quad i\partial_\varepsilon I(E, 0) \in \mathbb{R} \text{ when } E \in \text{neigh}(E_0, \mathbb{R}).$$

We now adopt the assumption (A7) so that the integral in (7.19) is non-vanishing for $(E, \varepsilon) = (E_0, 0)$ and in order to fix the ideas (possibly after replacing (ε, W) by $(-\varepsilon, -W)$) that

$$(7.21) \quad \int_{\alpha_\ell}^{\beta_\ell} (E_0 - V_0(x))^{-\frac{1}{2}} W(x) dx > 0,$$

so that

$$(7.22) \quad i\partial_\varepsilon I(E, 0) > 0 \text{ for } E \in \text{neigh}(E_0, \mathbb{R}).$$

Let $I_0 = I(E_0, 0) \in \mathbb{R}$. In view of the first part of (7.20), the map $I(\cdot, \varepsilon) : \text{neigh}(E_0, \mathbb{C}) \rightarrow \text{neigh}(I_0, \mathbb{C})$ is bijective for $\varepsilon \in \text{neigh}(0, \mathbb{R})$ with an inverse $K(\cdot, \varepsilon) : \text{neigh}(I_0, \mathbb{C}) \rightarrow \text{neigh}(E_0, \mathbb{C})$ such that $K(\iota, \varepsilon)$ is holomorphic in (ι, ε) . We also know that $K(\iota, 0)$ is real when ι is real. The property $\tilde{I}^* = \tilde{I}$ implies that $\tilde{I}(E, \varepsilon)$ is real when $\varepsilon = 0$ and since $\tilde{I} = I + \mathcal{O}(h^2)$, we see that $\tilde{I}(\cdot, \varepsilon)$ has a local inverse \tilde{K} with the same properties as K . Further, $\tilde{K} = K + \mathcal{O}(h^2)$ has a complete asymptotic expansion in powers of h in the space of holomorphic functions defined in a neighborhood of $(I_0, 0)$.

The zeros of the factor $\cos(\tilde{I}/h)$ are given by

$$(7.23) \quad \tilde{I}(E, \varepsilon) = \left(k + \frac{1}{2}\right) \pi h,$$

for $k \in \mathbb{Z}$ such that $(k + \frac{1}{2}) \pi h$ belongs to a neighborhood of I_0 . (The classical action for the left potential well is equal to $2I$, so we recognize the Bohr-Sommerfeld quantization condition $2\tilde{I}(E, \varepsilon) = (k + 1/2)2\pi h$.) They are situated on the real-analytic curve

$$(7.24) \quad \tilde{\Gamma}(\varepsilon) = \{E \in \text{neigh}(E_0, \mathbb{C}); \tilde{I}(E, \varepsilon) \in \mathbb{R}\}.$$

Alternatively, the zeros are of the form

$$(7.25) \quad \tilde{E}_k = \tilde{K}((k + 1/2)\pi h, \varepsilon),$$

and the curve (7.24) is of the form $\tilde{\Gamma}(\varepsilon) = \tilde{K}(\text{neigh}(0, \mathbb{R}), \varepsilon)$.

The curve $\tilde{\Gamma}$ can also be represented in the form

$$\tilde{\Gamma} : \text{Im } E = \tilde{g}(\text{Re } E, \varepsilon),$$

where

$$\tilde{g}(t, \varepsilon) \sim g(t, \varepsilon) + hg_1(t, \varepsilon) + \dots,$$

and

$$\Gamma : \text{Im } E = g(\text{Re } E, \varepsilon)$$

is the curve, determined by the condition $I(E, \varepsilon) \in \mathbb{R}$. We know that $\tilde{\Gamma}, \Gamma$ are real segments when $\varepsilon = 0$, so

$$\tilde{g}, g = \mathcal{O}(\varepsilon).$$

Writing

$$\text{Im } I(\text{Re } E + ig(\text{Re } E, \varepsilon), \varepsilon) = 0,$$

and differentiating with respect to ε at $\varepsilon = 0$, we get

$$\partial_\varepsilon g(\text{Re } E, 0) = \frac{i\partial_\varepsilon I}{\partial_E I}(\text{Re } E, 0) > 0.$$

Hence, by Taylor expansion,

$$g(\text{Re } E, \varepsilon) = \frac{i\partial_\varepsilon I}{\partial_E I}(\text{Re } E, 0)\varepsilon + \mathcal{O}(\varepsilon^2).$$

It follows that

$$\tilde{g}(\text{Re } E, \varepsilon) = \left(\frac{i\partial_\varepsilon I}{\partial_E I}(\text{Re } E, 0) + \mathcal{O}(h^2) \right) \varepsilon + \mathcal{O}(\varepsilon^2).$$

Similarly, by differentiating the equation $\tilde{I}(\tilde{E}_k(\varepsilon), \varepsilon) = (k + 1/2)\pi h$ with respect to ε , we get

$$\partial_\varepsilon \tilde{E}_k(\varepsilon) = i \frac{i\partial_\varepsilon \tilde{I}}{\partial_E \tilde{I}}(\tilde{E}_k(\varepsilon), \varepsilon),$$

and again by Taylor expansion at $\varepsilon = 0$,

$$\begin{aligned} \tilde{E}_k(\varepsilon) &= \tilde{E}_k(0) + i \frac{i\partial_\varepsilon \tilde{I}}{\partial_E \tilde{I}}(\tilde{E}_k(0), 0) \varepsilon + \mathcal{O}(\varepsilon^2) \\ (7.26) \quad &= (E_k(0) + \mathcal{O}(h^2)) + i \left(\frac{i\partial_\varepsilon I}{\partial_E I}(\tilde{E}_k(0), 0) + \mathcal{O}(h^2) \right) \varepsilon + \mathcal{O}(\varepsilon^2) \end{aligned}$$

Here $\tilde{E}_k(0)$ and $E_k(0)$ are real and given by the Bohr-Sommerfeld conditions

$$\tilde{I}(\tilde{E}_k(0), 0) = (k + 1/2)\pi h, \quad I(E_k(0), 0) = (k + 1/2)\pi h.$$

The zeros of the second factor

$$\cos(\tilde{I}^\dagger/h)(E, \varepsilon) = \overline{\cos(\tilde{I}/h)(\bar{E}, \varepsilon)},$$

are given by $E = \overline{\tilde{E}_k(\varepsilon)}$ and they are situated on the complex conjugate curve

$$\operatorname{Im} E = -\tilde{g}(\operatorname{Re} E, \varepsilon).$$

We next make an exponential localization of the zeros of f . We have,

$$|\cos z| \asymp \min(\operatorname{dist}(z, (\mathbb{Z} + 1/2)\pi), 1)e^{|\operatorname{Im} z|},$$

so for $E \in \operatorname{neigh}(E_0, \mathbb{C})$,

$$|\cos(\tilde{I}/h)| \asymp \min\left(\frac{1}{h}\operatorname{dist}(E, \{\tilde{E}_k\}), 1\right)e^{|\operatorname{Im} \tilde{I}|/h}.$$

Since $\tilde{I} = I + \mathcal{O}(h^2)$, we get

$$(7.27) \quad |\cos(\tilde{I}/h)| \asymp \min\left(\frac{1}{h}\operatorname{dist}(E, \{\tilde{E}_k\}), 1\right)e^{|\operatorname{Im} I|/h}.$$

Similarly,

$$(7.28) \quad |\cos(\tilde{I}^\dagger/h)| \asymp \min\left(\frac{1}{h}\operatorname{dist}(E, \{\overline{\tilde{E}_k}\}), 1\right)e^{|\operatorname{Im} I^\dagger|/h},$$

$$(7.29) \quad |\sin I/h| \leq 2e^{|\operatorname{Im} I|/h},$$

and

$$(7.30) \quad |\sin I^\dagger/h| \leq 2e^{|\operatorname{Im} I^\dagger|/h}.$$

We conclude that $f(E, \varepsilon) \neq 0$ when

$$|\cos(\tilde{I}/h) \cos(\tilde{I}^\dagger/h)| \gg e^{-2\operatorname{Re} J/h} |\sin(I/h) \sin(I^\dagger/h)|$$

and that this holds when

$$(7.31) \quad \min \left(\frac{1}{h} \text{dist} (E, \{\tilde{E}_k\}), 1 \right) \min \left(\frac{1}{h} \text{dist} (E, \{\overline{\tilde{E}_k}\}), 1 \right) \gg e^{-2 \text{Re } J(E, \varepsilon)/h}.$$

Thus if $C > 0$ is large enough, then $f(E, \varepsilon) \neq 0$ when

$$(7.32) \quad E \notin \bigcup_k D(\tilde{E}_k, Che^{-\text{Re } J(E, \varepsilon)/h}) \cup \bigcup_k D(\overline{\tilde{E}_k}, Che^{-\text{Re } J(E, \varepsilon)/h}).$$

Now we observe that for any $\hat{E} \in \text{neigh}(E_0, \mathbb{C})$,

$$\begin{aligned} E \in D(\hat{E}, Che^{-\text{Re } J(E, \varepsilon)/h}) &\implies E \in D(\hat{E}, 2Che^{-\text{Re } J(\hat{E}, \varepsilon)/h}), \\ E \in D(\hat{E}, 2Che^{-\text{Re } J(E, \varepsilon)/h}) &\implies E \in D(\hat{E}, Che^{-\text{Re } J(\hat{E}, \varepsilon)/h}). \end{aligned}$$

After doubling the constant in (7.32), we conclude that

$$(7.33) \quad f^{-1}(0, \varepsilon) \subset \bigcup_k D(\tilde{E}_k, Che^{-\text{Re } J(\tilde{E}_k, \varepsilon)/h}) \cup \bigcup_k D(\overline{\tilde{E}_k}, Che^{-\text{Re } J(\tilde{E}_k, \varepsilon)/h}).$$

If $E \in D(\tilde{E}_k, Che^{-\text{Re } J(\tilde{E}_k)/h})$ and if

$$(7.34) \quad \varepsilon \gg he^{-\text{Re } J(\tilde{E}_k)/h},$$

then $\text{dist}(E, \{\overline{\tilde{E}_k}\}) \asymp \varepsilon$, and from (7.31) we conclude that $f(E, \varepsilon) \neq 0$ if

$$(7.35) \quad \frac{1}{h} \text{dist}(E, \tilde{E}_k) \min \left(\frac{\varepsilon}{h}, 1 \right) \gg e^{-2 \text{Re } J(\tilde{E}_k, \varepsilon)/h}.$$

Thus, the zeros of f in $D(\tilde{E}_k, Che^{-\text{Re } J(\tilde{E}_k)/h})$ are contained in

$$D \left(\tilde{E}_k, \frac{Ch}{\min(\varepsilon/h, 1)} e^{-2 \text{Re } J(\tilde{E}_k, \varepsilon)/h} \right).$$

If we drop the assumption (7.34), we have

$$(7.36) \quad \begin{aligned} &f^{-1}(0, \varepsilon) \cap D(\tilde{E}_k, Che^{-\text{Re } J(\tilde{E}_k, \varepsilon)/h}) \\ &\subset D \left(\tilde{E}_k, Ch \min \left(1, \max(h/\varepsilon, 1) e^{-\text{Re } J(\tilde{E}_k, \varepsilon)/h} \right) e^{-\text{Re } J(\tilde{E}_k, \varepsilon)/h} \right). \end{aligned}$$

The same discussion is valid with \widetilde{E}_k replaced by $\overline{\widetilde{E}_k}$ and we get the following improvement of (7.33):

$$(7.37) \quad f^{-1}(0, \varepsilon) \subset \bigcup_k D\left(\widetilde{E}_k, r(\widetilde{E}_k, \varepsilon)\right) \cup \bigcup_k D\left(\overline{\widetilde{E}_k}, r\left(\overline{\widetilde{E}_k}, \varepsilon\right)\right),$$

where

$$(7.38) \quad r(E, \varepsilon) = Ch \min\left(1, \max(h/\varepsilon, 1)e^{-\operatorname{Re} J(E, \varepsilon)/h}\right) e^{-\operatorname{Re} J(E, \varepsilon)/h}.$$

By inserting a deformation parameter $\theta \in [0, 1]$ in front of the second term in the last expression for f in (7.14), we will not change the localization (7.37) of the zeros and the number of such zeros in each connected component of the set in the right hand side of that inclusion is independent of θ . It follows that

- when these discs are disjoint, $f(\cdot, \varepsilon)$ has precisely one zero in each of $D\left(\widetilde{E}_k, r\left(\widetilde{E}_k, \varepsilon\right)\right)$ and $D\left(\overline{\widetilde{E}_k}, r\left(\overline{\widetilde{E}_k}, \varepsilon\right)\right)$.
- in general $f(\cdot, \varepsilon)$ has precisely 2 zeros in

$$D\left(\widetilde{E}_k, r\left(\widetilde{E}_k, \varepsilon\right)\right) \cup D\left(\overline{\widetilde{E}_k}, r\left(\overline{\widetilde{E}_k}, \varepsilon\right)\right).$$

From the first of these observations, (7.33), (7.26) and the fact that

$$(7.39) \quad \frac{i\partial_\varepsilon I}{\partial_E I}(E, 0) > 0 \text{ when } E \text{ is real,}$$

we get

Proposition 7.1 *Assume (7.21) for $E \in \operatorname{neigh}(E_0, \mathbb{R})$ and that ε is real and*

$$1 \gg |\varepsilon| \geq h e^{-(\operatorname{Re} J(E_0) - 1/C)/h}$$

for some positive constant C . Then the eigenvalues in $\operatorname{neigh}(E_0, \mathbb{C})$ are simple and non-real of the form $z_k(\varepsilon; h)$, $\overline{z_k(\varepsilon; h)}$, $k \in \mathbb{Z}$, where

$$z_k = \widetilde{E}_k(\varepsilon; h) + \mathcal{O}(h) e^{-\operatorname{Re} J(\widetilde{E}_k, \varepsilon)/h}$$

and we recall (7.26), (7.25). The term $\mathcal{O}(h) e^{-\operatorname{Re} J(\widetilde{E}_k, \varepsilon)/h}$ can be replaced by $\mathcal{O}(r(\widetilde{E}_k, \varepsilon))$, where $r(E, \varepsilon)$ is defined in (7.38).

It remains to make a more detailed study, when

$$|\varepsilon| \leq h e^{-(\operatorname{Re} J(E_0) - 1/C)/h},$$

and for that we shall view $\tilde{E}_k(0; h)$ as the nondegenerate local minima of $f_0(E, 0)$, $E \in \operatorname{neigh}(E_0, \mathbb{R})$, where we put for $0 \leq \theta \leq 1$,

$$(7.40) \quad f_\theta(E, \varepsilon) = \cos(\tilde{I}/h) \cos(\tilde{I}^\dagger/h) - \frac{\theta}{4} e^{-2\tilde{J}/h} \sin(I/h) \sin(I^\dagger/h),$$

so that $f_1 = f$ in (7.14). Using that $f_\theta^* = f_\theta$ and $f_\theta^\dagger = f_\theta$ we see that for real E

- f_θ is real-valued,
- f_θ is an even function of ε .

Write

$$f_0 = g(E, \varepsilon) g^\dagger(E, \varepsilon), \quad g(E, \varepsilon) = \cos(\tilde{I}/h) = g^*(E, \varepsilon).$$

Let $E_c(0)$ be a (real) zero of $g(E, 0)$, so that $E_c(0) = \tilde{E}_k(0)$ for some $k \in \mathbb{Z}$. For $\varepsilon = 0$, we have $f_0 = g(E, 0)^2 \geq 0$ and $E_c(0)$ is therefore a nondegenerate local minimum of f_0 with $f_0(E_c(0), 0) = 0$. Extend $E_c(0)$ to an analytic family $E_c(\varepsilon)$ of critical points of $f_0(\cdot, \varepsilon)$:

$$(7.41) \quad \partial_E f_0(E_c(\varepsilon), \varepsilon) = 0.$$

We have for real E :

$$\partial_E f_0(E, \varepsilon) = 2 \operatorname{Re}(\partial_E g(E, \varepsilon) \overline{g(E, \varepsilon)}),$$

and differentiating this once more and putting $\varepsilon = 0$, $E = E_c(0)$, we get

$$\partial_E^2 f_0(E_c(0), 0) = 2 \partial_E g(E_c(0), 0) \overline{\partial_E g(E_c(0), 0)} = 2 (\partial_E g(E_c(0), 0))^2,$$

i.e.

$$(7.42) \quad \begin{aligned} h^2 \partial_E^2 f_0(E_c(0), 0) &= 2 \left(\sin(\tilde{I}(E_c(0), 0)/h) \right)^2 \left(\partial_E \tilde{I}(E_c(0), 0) \right)^2 \\ &= 2 \left(\partial_E \tilde{I}(E_c(0), 0) \right)^2, \end{aligned}$$

where the last identity follows from the fact that $\cos \tilde{I}(E_c(0), 0)/h = 0$.

Differentiating (7.41), we get

$$(\partial_E^2 f_0) \partial_\varepsilon E_c + \partial_\varepsilon \partial_E f_0 = 0.$$

Here we recall that when E is real, $f_0(E, \varepsilon)$ and $\partial_E f_0(E, \varepsilon)$ are even functions of ε and hence $\partial_\varepsilon \partial_E f_0(E, 0) = 0$. It follows that

$$(7.43) \quad (\partial_\varepsilon \partial_E f_0)(E_c(0), 0) = 0,$$

$$(7.44) \quad \partial_\varepsilon E_c(0) = 0.$$

Using this, we get

$$\begin{aligned} & (\partial_\varepsilon)_{\varepsilon=0}^2 (f_0(E_c(\varepsilon), \varepsilon)) \\ &= (\partial_\varepsilon)_{\varepsilon=0} \left(\underbrace{(\partial_E f_0)(E_c(\varepsilon), \varepsilon)}_{=0} \partial_\varepsilon E_c(\varepsilon) + (\partial_\varepsilon f_0)(E_c(\varepsilon), \varepsilon) \right) \\ &= (\partial_\varepsilon)^2 f_0(E_c(0), 0) + \underbrace{(\partial_E \partial_\varepsilon f_0)(E_c(\varepsilon), \varepsilon)}_{=0} \underbrace{\partial_\varepsilon E_c(0)}_{=0} \\ &= 2 |\partial_\varepsilon g(E_c(0), 0)|^2. \end{aligned}$$

Thus,

$$\begin{aligned} (7.45) \quad & h^2 (\partial_\varepsilon)_{\varepsilon=0}^2 (f_0(E_c(\varepsilon), \varepsilon)) = 2 \left(\sin \tilde{I}(E_c(0), 0)/h \right)^2 \left| (\partial_\varepsilon \tilde{I})(E_c(0), 0) \right|^2 \\ &= 2 \left| (\partial_\varepsilon \tilde{I})(E_c(0), 0) \right|^2. \end{aligned}$$

We next extend $E_c(\varepsilon)$ to an analytic function $E_c(\varepsilon, \theta)$ determined by the conditions $E_c(\varepsilon, 0) = E_c(\varepsilon)$,

$$(7.46) \quad \partial_E f_\theta(E_c(\varepsilon, \theta), \varepsilon) = 0.$$

It will be convenient to restrict the attention to a window of size $\mathcal{O}(h)$:

$$(7.47) \quad E = E_1 + hF, \quad \varepsilon = h\tilde{\varepsilon},$$

where $E_1 \in \text{neigh}(E_0, \mathbb{R})$ is a parameter and $F \in \text{neigh}(0, \mathbb{C})$, $\tilde{\varepsilon} \in \text{neigh}(0, \mathbb{R})$ are rescaled variables. It will also be convenient to have a “Floquet parameter” $\kappa \in \mathbb{R}$ and introduce the following extension of (7.40):

$$(7.48) \quad f_\theta(E, \varepsilon, \kappa) = \cos\left(\frac{\tilde{I}}{h} - \kappa\right) \cos\left(\frac{\tilde{I}^\dagger}{h} - \kappa\right) - \frac{\theta}{4} e^{-2\tilde{J}/h} \sin\left(\frac{I}{h} - \kappa\right) \sin\left(\frac{I^\dagger}{h} - \kappa\right),$$

which coincides with $f_\theta(E, \varepsilon)$, when $\kappa \in \pi\mathbb{Z}$. Again, f_θ is real-valued when E is real and an even function of ε . If we let $E_c(\varepsilon, \kappa, \theta)$ denote a local minimum of $f_\theta(\cdot, \varepsilon, \kappa)$, then (7.42), (7.43), (7.44) extend naturally to the case $\theta = 0$. Writing

$$\kappa = \tilde{\kappa} + I(E_1, 0)/h,$$

we get

$$(7.49) \quad f_\theta = \tilde{f}_\theta(F, \tilde{\varepsilon}, \tilde{\kappa}; h) = a(F, \tilde{\varepsilon}, \tilde{\kappa}; h) + \theta e^{-2J(E_1, 0)/h} b(F, \tilde{\varepsilon}, \tilde{\kappa}; h),$$

where a, b are classical symbols of order 0 in h :

$$a \sim a_0 + ha_1 + \dots, \quad b \sim b_0 + hb_1 + \dots$$

The critical points with respect to F are nondegenerate and their number is uniformly bounded. They have asymptotic expansions in powers of h of the form,

$$F_c(\tilde{\varepsilon}, \tilde{\kappa}, \theta; h) \sim F_c^0(\tilde{\varepsilon}, \tilde{\kappa}, \theta e^{-2J(E_1, 0)/h}) + h F_c^1(\tilde{\varepsilon}, \tilde{\kappa}, \theta e^{-2J(E_1, 0)/h}) + \dots$$

which gives

$$(7.50) \quad F_c(\tilde{\varepsilon}, \tilde{\kappa}, \theta; h) = F_c^1(\tilde{\varepsilon}, \tilde{\kappa}; h) + \theta e^{-2J(E_1, 0)/h} F_c^2(\tilde{\varepsilon}, \tilde{\kappa}, \theta; h),$$

where F_c^k are classical symbols of order 0 in h and also holomorphic functions. Notice that the terms in the asymptotic expansion of F_c^2 in powers of h are independent of θ . $E_c = E_1 + h F_c$ will be a critical point of $f_\theta(\cdot, \varepsilon)$ in (7.40) when $\kappa \in \pi\mathbb{Z}$, i.e. when

$$(7.51) \quad \tilde{\kappa} \equiv -\frac{I(E_1, 0)}{h} \pmod{\pi\mathbb{Z}}.$$

It follows from (7.50) that

$$F_c(\tilde{\varepsilon}, \tilde{\kappa}, \theta; h) = F_c(\tilde{\varepsilon}, \tilde{\kappa}, 0; h) + \mathcal{O}(1)\theta e^{-2J(E_1, 0)/h},$$

and hence that

$$(7.52) \quad E_c(\varepsilon, \kappa, \theta) = E_c(\varepsilon, \kappa, 0) + \mathcal{O}(h)\theta e^{-2J(E_1, 0)/h}.$$

To evaluate the critical value $f_\theta(E_c(\varepsilon, \kappa, \theta), \varepsilon, \kappa) =: f_\theta^c(\varepsilon, \kappa)$ for $\theta = 1$, we notice that

$$\begin{aligned} \partial_\theta(f_\theta(\varepsilon, \kappa)) &= (\partial_\theta f_\theta)(E_c(\varepsilon, \kappa, \theta)) \\ &= -\frac{1}{4} \left(e^{-2\tilde{J}/h} \sin\left(\frac{I}{h} - \kappa\right) \sin\left(\frac{I^\dagger}{h} - \kappa\right) \right) (E_c(\varepsilon, \kappa, \theta), \varepsilon, \kappa) \\ &= -\frac{1}{4} e^{-2\tilde{J}(E_c(0, \kappa, 0), 0)} \times \\ &\quad \left[\left(\sin\left(\frac{I}{h} - \kappa\right) \right)^2 (E_c(0, \kappa, 0), 0, \kappa) + \mathcal{O}(1) \left(\theta e^{-2\operatorname{Re} J(E_1, 0)/h} + \frac{|\varepsilon|}{h} \right) \right]. \end{aligned}$$

Here, we use that

$$\sin\left(\frac{\tilde{I}}{h} - \kappa\right) (E_c(0, \kappa, 0), 0, \kappa) = \pm 1, \quad \sin\left(\frac{I}{h} - \kappa\right) = \sin\left(\frac{\tilde{I}}{h} - \kappa\right) + h$$

and integrate from $\theta = 0$ to $\theta = 1$, to get

$$(7.53) \quad \begin{aligned} f_1^c(\varepsilon, \kappa) &= f_0^c(\varepsilon, \kappa) \\ &- \frac{1}{4} e^{-2J(E_c(0, \kappa, 0), 0)/h} \left(1 + \mathcal{O}\left(e^{-2\operatorname{Re} J(E_1, 0)/h} + \frac{|\varepsilon|}{h} + \mathcal{O}(h) \right) \right). \end{aligned}$$

Now, return to the window (7.47), where $f_\theta = \tilde{f}_\theta(F, \tilde{\varepsilon}, \tilde{\kappa}; h)$ is given by (7.49) and the critical point F_c is as in (7.50). We have with $\theta = 1$ (and suppressing the corresponding subscript 1)

$$(7.54) \quad f^c(\varepsilon, \kappa; h) = \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) = g_1(\tilde{\varepsilon}, \tilde{\kappa}; h) + g_2(\tilde{\varepsilon}, \tilde{\kappa}; h) e^{-2J(E_c(0, \kappa, 0), 0)/h},$$

where g_j are classical symbols of order 0 in h . (We first get this with $J(E_1, 0)/h$ in the exponent, but the replacement by $J(E_c(0, \kappa, 0), 0)$ does not modify the general structure of the formula.) (7.53) shows that

$$(7.55) \quad g_1(0, \tilde{\kappa}; h) = 0, \quad g_2(0, \tilde{\kappa}) = -\frac{1}{4},$$

where $g_{j,0}$ is the leading term in the asymptotic expansion of g_j .

From (7.45), we deduce that

$$(7.56) \quad \partial_{\tilde{\varepsilon}}^2 g_{1,0}(0, \tilde{\kappa}) = 2|\partial_{\varepsilon} I(E_1, 0)|^2 > 0.$$

Combining (7.54), (7.55), (7.56), we get by Taylor expansion,

$$(7.57) \quad \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) = g_2(0, \tilde{\kappa}; h) e^{-2J(E_c(0, \kappa, 0), 0)/h} + k(\tilde{\varepsilon}, \tilde{\kappa}; h) \tilde{\varepsilon}^2,$$

where k is a symbol of order 0 in h , holomorphic in the other variables, even in $\tilde{\varepsilon}$ and satisfying $k(0, \tilde{\kappa}; 0) = |\partial_{\varepsilon} I(E_1, 0)|^2$. $\tilde{f}^c(\cdot, \kappa; h)$ has precisely two zeros in a neighborhood 0 which are real and of the form $\pm \tilde{\varepsilon}_c(\kappa; h)$, where

$$(7.58) \quad \tilde{\varepsilon}_c(\kappa; h) = \ell(\tilde{\kappa}; h) e^{-J(E_c(0, \kappa, 0), 0)/h},$$

and ℓ is a symbol of order 0 with leading term

$$\ell_0(\tilde{\kappa}) = \frac{1}{2|\partial_{\varepsilon} I(E_1, 0)|}.$$

Using that our functions are holomorphic in $\tilde{\varepsilon}$, $\tilde{\kappa}$, we see that

$$(7.59) \quad \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) = m(\tilde{\varepsilon}, \tilde{\kappa}; h) (\tilde{\varepsilon}^2 - \tilde{\varepsilon}_c(\tilde{\kappa}; h)^2),$$

where m is holomorphic in $\tilde{\varepsilon}$, $\tilde{\kappa}$ and a symbol of order 0 in h with leading term $m_0(\tilde{\varepsilon}, \tilde{\kappa})$, satisfying

$$(7.60) \quad m_0(0, \tilde{\kappa}) = |\partial_{\varepsilon} I(E_1, 0)|.$$

(7.42) can be extended to the κ -dependent case:

$$(7.61) \quad (h^2 \partial_E^2 f_0)(E_c(0, \kappa, 0), \kappa, 0) = 2(\partial_E \tilde{I}(E_c(0, \kappa, 0)))^2.$$

This implies that

$$(7.62) \quad (\partial_F^2 \tilde{f}_1)(F_c, \tilde{\varepsilon}, \tilde{\kappa}; h) = (\partial_E I(E_c(0, \kappa, 0), 0))^2 + \mathcal{O}(h),$$

where the remainder has a complete asymptotic expansion in powers of h . By Taylor expansion,

$$(7.63) \quad \tilde{f}_1(F, \tilde{\varepsilon}, \tilde{\kappa}; h) = \tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h) + q(F, \tilde{\varepsilon}, \tilde{\kappa}; h) (F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h))^2,$$

where $q > 0$ is a symbol of order 0 and

$$(7.64) \quad q(F_c, 0, \tilde{\kappa}; 0) = 2(\partial_E \tilde{I}(E_c(0, \kappa, 0), 0))^2.$$

$\tilde{f}(\cdot, \tilde{\varepsilon}, \tilde{\kappa}; h)$ has two zeros in a small neighborhood of F_c when counted with their multiplicity:

- When $|\tilde{\varepsilon}| < \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ the zeros are real and simple, given by

$$(7.65) \quad q(F, \tilde{\varepsilon}, \tilde{\kappa}; h)^{\frac{1}{2}}(F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h)) = \pm(-\tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h))^{\frac{1}{2}}$$

- When $|\tilde{\varepsilon}| = \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ we have a double zero,

$$(7.66) \quad F = F_c.$$

- When $|\tilde{\varepsilon}| > \tilde{\varepsilon}_c(\tilde{\kappa}; h)$ the zeros are non-real and simple and complex conjugate to each other, given by

$$(7.67) \quad q(F, \tilde{\varepsilon}, \tilde{\kappa}; h)^{\frac{1}{2}}(F - F_c(\tilde{\varepsilon}, \tilde{\kappa}, 1; h)) = \pm i(\tilde{f}^c(\tilde{\varepsilon}, \tilde{\kappa}; h))^{\frac{1}{2}}.$$

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